Influence of Small Impurities on Low-Energy Electron Dynamics in Two-Dimensional Microscopic Bounded Region

T. Shigehara¹, M. Yokoyama¹, H. Mizoguchi¹, T. Mishima¹ and Taksu Cheon²

¹Department of Information and Computer Sciences, Saitama University
Shimo-Okubo 255, Urawa, Saitama 338-8570, JAPAN
Phone: +81-48-858-9035, Fax: +81-48-858-3716, E-MAIL: sigehara@ics.saitama-u.ac.jp

²Laboratory of Physics, Kochi University of Technology
Tosa Yamada, Kochi 782-8502, JAPAN
Phone: +81-8875-7-2302, Fax: +81-8875-7-2320, E-MAIL: cheon@mech.kochi-tech.ac.jp

Abstract—In order to give some insight into a role of small impurities on the electron motion in microscopic devices, we examine from a general viewpoint, the effect of small obstacles on a particle motion at low energy inside microscopic bounded regions. It will be shown that the obstacles disturb the electron motion only if they are weakly attractive.

I. Introduction

The recent progress of microscopic technology makes it possible to construct extremely pure structures which are expected to be a main component of promising quantum devices such as a single-electron memory. However, real systems are not free from small impurities which might possibly affect the electron motion inside. It is an urgent problem to reveal the condition under which the wave function of the electron is substantially distorted by the small impurities. This is exactly our subject in this paper.

We here restrict ourselves to the case of spatial dimension two. We begin in Sect.2 with a simple but exactly solvable model where a pointlike particle with mass \( M \) freely moves in a two-dimensional bounded region which contains a pointlike scatterer inside. It is a well-known fact that the Dirac’s delta potential does not work in quantum mechanics in spatial dimension two. Based on the self-adjoint extension of a symmetric operator in functional analysis, however, we derive a suitable transition matrix for the system with a pointlike interaction. By examining the general feature of the eigenvalue equation for the system, we deduce the general condition under which the eigenfunctions are substantially affected by the pointlike scatterer. In Sect.3, we consider a quantum-mechanical one-body problem with the potential which has constant strength \( U_1 \) in a small but finite region of size \( \Omega \). The potential is expected to behave as pointlike at low energy where the electron wavelength is much larger than the range of the potential. Thus we can apply the findings for pointlike obstacles to such cases. Keeping the area \( \Omega \) small but finite-size, we show that the electron motion at the energy \( \omega \) is substantially distorted by the potential under the condition

\[
\left| \frac{1}{U_1 M \Omega} - \frac{1}{2 \pi} \ln(\omega M \Omega) \right| < \frac{\pi}{4}.
\]

This indicates that the small impurities influence the low-energy electron wave function only if they are weakly attractive. The validity of our conjecture is confirmed by numerical experiments. The current work is summarized in Sect.4.

II. The Case of Point Impurity

We first consider a quantum point particle of mass \( M \) moving freely in a two-dimensional bounded region \( S \). Let us denote the area of \( S \) by the same symbol. We impose the Dirichlet boundary condition so that wave functions vanish on the boundary of \( S \). The eigenvalues and the corresponding normalized eigenfunctions are denoted by \( E_n \) and \( \varphi_n(x) \) respectively;

\[
H_0\varphi_n(x) \equiv -\frac{\nabla^2}{2M}\varphi_n(x) = E_n\varphi_n(x).
\]

The Green’s function of the kinetic operator \( H_0 \) is written as

\[
G^{(0)}(x, y; \omega) = \sum_{n=1}^{\infty} \frac{\varphi_n(x)\varphi_n(y)}{\omega - E_n},
\]

where \( \omega \) is the energy variable. The average level density of the system is given by \( \rho_{av} = MS/2\pi \), which is energy-independent. We now place a single point impurity at \( x_1 \)
in the region \(S\). The most naive manner for this purpose is to define the impurity by using the Dirac’s \(\delta\) function of strength \(v_1\):

\[
H = H_0 + v_1 \delta(x - x_1).
\]

(4)

However, the Hamiltonian \(H\) is not mathematically sound. This can be seen from the eigenvalue equation of \(H\), which is reduced to

\[
\sum_{n=1}^{\infty} \frac{\varphi_n(x_1)^2}{\omega - E_n} = \tilde{v}_1^{-1}.
\]

(5)

Since the average level density \(\rho_{av}\) is constant in spatial dimension two, the infinite series does not converge.

One of the general schemes to handle the divergence is based on the self-adjoint extension theory of functional analysis. We first restrict the domain of \(H_0\), say \(D(H_0)\), to the functions which vanish at the location of the point impurity; \(H_{\mathbf{x}_1} = -\nabla^2/2M\), \(D(H_{\mathbf{x}_1}) = \{\psi \in D(H_0)|\psi(x_1) = 0\}\). By using integration by parts, it is easy to prove that the operator \(H_{\mathbf{x}_1}\) is symmetric (Hermitian). But it is not self-adjoint. Indeed, the eigenvalue equation \(H_\mathbf{x}_1 \psi_\omega = \omega \psi_\omega\) for the adjoint of \(H_\mathbf{x}_1\) has a solution for \(Im\omega \neq 0\) in \(\psi_\omega(x) = G^{(0)}(x, x_1; \omega)\). Since the deficiency indices of \(H_\mathbf{x}_1\) are \((1,1)\), \(H_\mathbf{x}_1\) has one-parameter family of self-adjoint extensions \(H_{\theta_1}\) \((0 \leq \theta_1 < 2\pi)\) which is regarded as the proper Hamiltonian for the system with a point impurity at \(x_1\). Following Zorbas, we can write down the Green’s function for \(H_{\theta_1}\) as

\[
G_{\theta_1}(\mathbf{x}, \mathbf{y}; \omega) = G^{(0)}(\mathbf{x}, \mathbf{y}; \omega) + G^{(0)}(\mathbf{x}, x_1; \omega)T_{\theta_1}(\omega)G^{(0)}(x_1, \mathbf{y}; \omega),
\]

(6)

where the transition matrix \(T_{\theta_1}\) is calculated by

\[
T_{\theta_1}(\omega) = \frac{1 - e^{-i\theta_1}}{(\omega - i\Lambda)c_{i\Lambda}(\omega) - e^{i\theta_1}(\omega + i\Lambda)c_{-i\Lambda}(\omega)},
\]

(7)

with

\[
c_{\pm i\Lambda}(\omega) = \int_S G^{(0)}(\mathbf{x}, \mathbf{x}_1; \omega)G^{(0)}(\mathbf{x}, \mathbf{x}_1; \pm i\Lambda)d\mathbf{x}.
\]

(8)

Here \(\Lambda > 0\) is an arbitrary scale mass. The eigenvalues of \(H_{\theta_1}\) are determined by \(T_{\theta_1}(\omega)^{-1} = 0\), which is reduced to

\[
G(\omega) = \tilde{v}_1^{-1},
\]

(9)

where

\[
G(\omega) = \sum_{n=1}^{\infty} \frac{\varphi_n(x_1)^2}{\omega - E_n} + \frac{E_n}{E_n^2 + \Lambda^2},
\]

(10)

\[
\tilde{v}_1^{-1} = \Lambda \cot \frac{\theta_1}{2} \sum_{n=1}^{\infty} \frac{\varphi_n(x_1)^2}{E_n^2 + \Lambda^2}.
\]

(11)

The constant \(\tilde{v}_1\) can be formally considered as the strength of the point impurity, the value of which ranges over the whole real number as \(0 \leq \theta_1 < 2\pi\). On any interval \((E_m, E_{m+1})\), the function \(G\) is monotonically decreasing, ranging over the whole real number. This means that the eigenvalue equation \(\varphi_n(x_1)^2\) has a single solution \(\omega_m\) on each interval for any \(\tilde{v}_1\). The eigenfunction of \(H_{\theta_1}\) corresponding to an eigenvalue \(\omega_m\) is given by

\[
\psi_m(x) \propto G^{(0)}(x, x_1; \omega_m) = \sum_{n=1}^{\infty} \frac{\varphi_n(x_1)}{\omega_m - E_n} \varphi_n(x).
\]

(12)

Based on the formulation described above, we deduce the condition for the appearance of the effect of point impurities on the particle motion. The first notice is that the average value of \(\varphi_n(x_1)^2\) among many \(n\) is constant; \(\langle \varphi_n(x_1)^2 \rangle \sim 1/\Lambda\). We thus recognize from (12) that if \(\omega_m \approx E_m\) (resp. \(E_{m+1}\) for some \(m\), then \(\psi_m \approx \varphi_m\) (resp. \(\psi_m \approx \varphi_{m+1}\)). This implies that a point impurity distorts the wave function if the eigenvalue \(\omega_m\) is located around the midpoint of the interval \((E_m, E_{m+1})\). For such \(\omega_m\), the value of \(G(\omega_m)\) can be estimated by using the principal integral, since the contributions on the summation of \(G\) from the terms with \(n \approx m\) cancel each other. We thus realize that the point impurity of formal strength \(\tilde{v}_1\) causes the wave function mixing mainly in the eigenstate with an eigenvalue \(\omega\) which satisfies

\[
|\tilde{v}_1^{-1} - \alpha \cdot P \int_0^{\infty} \left( \frac{1}{\omega - E} + \frac{E}{E^2 + \Lambda^2} \right) dE \leq \frac{\Delta}{2},
\]

(13)

with \(\alpha = \langle \varphi_n(x_1)^2 \rangle_{\rho_{av}} = M/2\pi\), leading to

\[
|\tilde{v}_1^{-1} - \frac{M}{2\pi} \ln \frac{\omega}{\Lambda} | \leq \frac{\Delta}{2}.
\]

(14)

The “width” \(\Delta\) of the strong coupling region is estimated by considering the variance of \(G\) linearized at \(\omega = (E_m + E_{m+1})/2\) on the interval \((E_m, E_{m+1})\):

\[
\Delta \simeq |G'(\omega)| \rho_{av}^{-1} \simeq \sum_{n=1}^{\infty} \frac{\left( \varphi_n(x_1)^2 \right)}{(\omega - E_n)^2} \rho_{av}^{-1}
\]

\[
\simeq \langle \varphi_n(x_1)^2 \rangle \sum_{n=1}^{\infty} \frac{2\rho_{av}^{-1}}{(n - 1/2)^2 \rho_{av}^{-1}}
\]

\[
= \pi^2 \langle \varphi_n(x_1)^2 \rangle \rho_{av} = \frac{\pi M}{2}.
\]

(15)

The third equality follows from the approximation that the unperturbed eigenvalues are distributed with a mean interval \(\rho_{av}^{-1}\) in the whole energy region.
We can summarize the findings as follows: The effect of a point impurity of formal coupling strength $\tilde{v}_1$ is substantial mainly in the eigenstates with eigenvalue $\omega$ such that
\begin{equation}
\tilde{v}_1^{-1} - \frac{M}{2\pi} \ln \frac{\omega}{\Lambda} \sim \frac{\pi M}{4} \tag{16}
\end{equation}
in two dimension. Numerical supports for the condition \ref{16} are shown in \ref{4}–\ref{6}.

III. The Case of Finite-Size Impurity

We have revealed the condition for the appearance of the effect of point impurities in the previous section. It should be noticed that the condition \ref{16} is written in terms of the formal strength $\tilde{v}_1$ as well as the scale mass $\Lambda$, either of which does not have a direct relation to the physical observables. It is realized, however, that both disappear in case of realistic finite-range impurities and the condition for the strong coupling can be described only in terms of the observables.

Suppose that a small but finite-size impurity of the area $\Omega$ is located around $\mathbf{x} = \mathbf{x}_1$ inside the region $S$. We describe the impurity in terms of a potential which has a constant strength in the region $\Omega$:
\begin{equation}
U(\mathbf{x}) = \begin{cases} 
U_1, & \mathbf{x} \in \Omega, \\
0, & \mathbf{x} \in S - \Omega.
\end{cases} \tag{17}
\end{equation}
We assume that the impurity has the same order of size, say $R$, in each spatial direction, and also assume that the size of the impurity is substantially smaller than that of the outer region; $\Omega \approx R^2 \ll S$. In this case, the impurity behaves as pointlike at low energy $\omega \ll E_{N(\Omega)}$, where $N(\Omega)$ is determined by $E_{N(\Omega)} \approx 1/\xi R^2 \approx 1/M\Omega$. Furthermore, the coupling of higher energy states than $E_{N(\Omega)}$ to the low-energy states is weak, since wave functions with wavelength shorter than $R$ oscillate within the impurity. This means that the low-energy states ($\omega \ll E_{N(\Omega)}$) can be described by the Hamiltonian \ref{3} with the $\delta$-potential of the coupling strength $v_1 \equiv U_1 \Omega$, together with a basis truncated at $E_{N(\Omega)}$. The truncation of basis is crucial for the present argument. As mentioned before, in two dimension, the $\delta$-potential is not well-defined in the full unperturbed basis. The finiteness of the impurity introduces an ultra-violet cut-off in a natural manner and as a result, the low-energy dynamics can be reproduced by the Hamiltonian \ref{3} within a suitably truncated basis.

The strength $v_1$ can be related to the formal strength $\tilde{v}_1$ as follows. Within the truncated basis $\{ \varphi_n(\mathbf{x}) | n = 1, 2, ..., N(\Omega) \}$, the eigenvalues of the Hamiltonian \ref{3} are determined by
\begin{equation}
\sum_{n=1}^{N(\Omega)} \frac{\varphi_n(\mathbf{x}_1)^2}{\omega - E_n} = v_1^{-1}. \tag{18}
\end{equation}
From \ref{3}, \ref{3} and \ref{13}, we obtain
\begin{align}
\tilde{v}_1^{-1} &= v_1^{-1} + \sum_{n=1}^{N(\Omega)} \frac{\varphi_n(\mathbf{x}_1)^2}{E_n^2 + \Lambda^2} \\
&\quad + \sum_{n=N(\Omega)+1}^{\infty} \frac{\varphi_n(\mathbf{x}_1)^2}{\omega - E_n + E_n^2 + \Lambda^2} \tag{19}.
\end{align}

The equation \ref{19} gives an exact relation between $\tilde{v}_1$ and $v_1$. In order to gain further insight on \ref{19}, we take the same approximation by integrals as in the previous section:
\begin{equation}
\tilde{v}_1^{-1} \approx v_1^{-1} + \alpha \left\{ \int_0^{E_{N(\Omega)}} \frac{E}{E^2 + \Lambda^2} dE \\
+ \int_{E_{N(\Omega)}}^{\infty} \left( \frac{1}{\omega - E} + \frac{E}{E^2 + \Lambda^2} \right) dE \right\}. \tag{20}
\end{equation}
Inserting \ref{20} into \ref{13}, we obtain the strong coupling condition for the finite-size impurity;
\begin{equation}
\left| v_1^{-1} - \alpha \cdot P \int_0^{E_{N(\Omega)}} \frac{dE}{\omega - E} \right| \approx \frac{\Lambda}{2} \approx \frac{\pi M}{4}. \tag{21}
\end{equation}
This is exactly the condition for the eigenvalue equation \ref{13} to have a solution $\omega$ around the midpoint on some interval $(E_m, E_{m+1})$. Performing the integration in \ref{21} and noticing $v_1 = U_1 \Omega$, $\alpha \approx M/2\pi$, we have the condition \ref{13} for $\omega \ll E_{N(\Omega)} \approx 1/M\Omega$. An arbitrary scale mass $\Lambda$ disappears and \ref{13} is written in terms of the observables. This gives the general condition for the appearance of the effect of finite-size impurities on the electron motion in two-dimensional microscopic bounded regions: At low energy where finite-size impurities can be regarded as pointlike ($\omega \ll 1/M\Omega$), the electron (of effective mass $M$) is most strongly coupled to finite-size ($\simeq \Omega$) impurities of potential height $U_1$ under the condition \ref{13}.

The most important indication of \ref{13} is that the effect of finite-size impurities at low energy appears most strongly when it is weakly attractive. In order to confirm this numerically, we examine the wave function in a two-dimensional rectangular region with a small rectangular impurity inside \ref{3}. In the following, we set the scale mass $\Lambda = 1$ without losing generality. The unperturbed eigenvalues and the corresponding normalized eigenfunctions without the impurity are given by
\begin{equation}
E_{m,n} = \frac{1}{2M} \left\{ \left( \frac{m\pi}{l_x} \right)^2 + \left( \frac{n\pi}{l_y} \right)^2 \right\}, \tag{22}
\end{equation}
Dependence of the eigenfunction on the nature of the impurity: (a) strong repulsion ($v_1 = 10$), (b) strong attraction ($v_1 = -3.33$), and (c) weak attraction ($v_1 = -0.25$). The eigenvalue $\omega$ of each state is (a) $\omega = 4.93$, (b) $\omega = 4.43$, and (c) $\omega = 5.63$, respectively. The location of the impurity is denoted by a small rectangle.

and

$$\varphi_{m,n}(x, y) = \sqrt{\frac{4}{l_x l_y}} \sin \frac{m \pi x}{l_x} \sin \frac{n \pi y}{l_y},$$

with $m, n = 1, 2, 3, \ldots$, respectively. We take the side-lengths of the (outer) rectangle as $(l_x, l_y) = (\pi/3, 3/\pi)$. The mass of the particle is set to $M = 2\pi$, leading to $\rho_{av} = 1$. A small rectangular impurity with side-lengths $(\delta l_x, \delta l_y) = (3.53830 \times 10^{-2}, 3.14023 \times 10^{-2})$ (area $\Omega = 1/900$) is placed at $x_1 = (0.622482, 0.275835)$ such that the sides of the inner and outer rectangles are parallel to each other.

Fig.1 shows the dependence of the wave function on the nature of the impurity in the low-energy region. All the eigenstates are located between the unperturbed energies $E_{1,2} = 4.16$ and $E_{2,2} = 6.31$. Thus, the main components of each wave function are expected to be $\varphi_{1,2}$ and $\varphi_{2,2}$. In both cases of strong repulsion (a) and strong attraction (b), the wave function is dominated only by a single component $\varphi_{1,2}$ except around the small impurity, which is denoted by a small rectangle in Fig.1. It is worthy to note that the direct measure of the strength of the impurity is given by the ratio between $v_1 = U_1 \Omega$ and the mean level spacing $\rho_{av}^{-1}$. Since $\rho_{av} = 1$, Both (a) and (b) indeed correspond to the strong force. Conversely, the mixture of the unperturbed eigenfunctions occurs in case of weak attraction (c), for which the strong coupling condition $1/U_1 M \Omega \simeq \ln(\omega M \Omega)/2\pi$ is satisfied with high degree of accuracy. These results confirm the validity of the prediction (1). For details, the readers are referred to [1].

IV. Conclusion

We have discussed the effect of small impurities on the electron motion in two-dimensional microscopic bounded regions from a general perspective. The condition for the appearance of their effect is made clear in a quantitative manner. The equation (1) indicates the followings;

1. The effect of small impurities on the low-energy electron motion in two-dimensional microscopic bounded region appears when the potential is weakly attractive, while it can be neglected in case of strong force.
2. The strong coupling region is described by a logarithmically energy-dependent strip with an energy-independent width in the $\omega$ versus $U_1^{-1}$ plane. This means that the strength of the small impurities which affect the electron dynamics changes as the electron energy increases.

References

[1] S. Albeverio, F. Gesztesy, R. Høegh-Krohn, and H. Holden, “Solvable models in quantum mechanics,” Springer-Verlag, New York, 1988.
[2] M. Reed and B. Simon, “Methods of modern mathematical physics,” vol.2, “Fourier analysis, self-adjointness,” Academic Press, New York, 1975.
[3] J. Zorbas, J. Math. Phys., vol.21, no.4, pp.840–847, 1980.
[4] T. Shigehara, Phys. Rev. E, vol.50, no.6, pp.4357–4370, 1994.
[5] T. Shigehara, H. Mizoguchi, T. Mishima, and T. Cheon, Proc. International Symposium on Nonlinear Theory and its Applications, NOLTA’97, pp.441–444, Honolulu, Nov., 1997.
[6] T. Shigehara, H. Mizoguchi, T. Mishima, and T. Cheon, “Chaos induced by quantization,” IEICE Trans. Fundamentals, to be published.
[7] T. Shigehara and T. Cheon, Phys. Rev. E, vol.54, no.2, pp.1321–1331, 1996.