Analytical and numerical study of diffusion and localization of cold atoms in 3D optical speckles

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Abstract: This paper aims to study the diffusion and localization of cold atoms in three-dimensional (3D) optical speckles by using the theory of self-energy for \(N\) diffusers. In this paper, the Self-consistent Born approximation (SCBA) is used to study the diffusion and localization of cold atoms in an optical disordered speckles, while the spectral function is adopted to study the effect of the matter waves energy and the disorder amplitude on the behaviour of cold atoms. For this purpose, the models of SCBA and spectral function are computed by a numerical algorithm. The calculation of the latter quantity involves the application of Simpson’s integration methods. The diffusion and localization of a Bose–Einstein Condensate for First-order Born Approximation (FBA) and SCBA models are presented. In addition, the diffusion time and the mean free path between two diffusers are illustrated. Moreover, the effect of disorder amplitude and the scattering of matter waves in 3D disordered potentials are highlighted. In this study, the results show that the time response of cold atoms localization and metal–insulator transition in SCBA is faster and yields lower energy than the FBA approximation.

Keywords: Cold atoms; 3D optical speckles; First-order Born Approximation (FBA); Self-consistent Born approximation (SCBA); Spectral function

1. Introduction

Recently, most tasks performed in the society in which we live, such as administrative work, studies and media are oriented toward the Information and Communication Technology (ICT) [1, 2]. Indeed, the spread of COVID-19 pandemic across the world shows the importance of ICT in our lives. In fact, heads of government have fought this pandemic by allowing the telecommuting and by making studies, conferences and meetings remotely [3]. On the other hand, the devices of ICT have been integrated into homes, transportation tools and in various fields to build a smart society and to improve the infrastructure building [4, 5]. However, the efficiency of ICT devices, i.e., computers, GPS, the geostationary satellite is related to the accuracy of integrated sensors and the kind of oscillation clock used in them. For this purpose, many experiments and research have been performed to improve the efficiency of ICT devices by using the properties of cold atoms in the constitution of these devices [6].

In the early 1990s, the first atom interferometers opened a new branch of research in which the physicists researchers have been able to use the ultra-cold atoms to improve the quantum devices and to increase the efficiency and the precision of digital sensors [7, 8]. For this purpose, several research papers have been published in the last 20 years to present the new challenges of ultra-cold atoms that could help other researchers find more accurate sensors. In this regard, a review of some sustainable developments that have been achieved in the last 20 years regarding matter-wave Sagnac interferometers is presented in [9]. In addition, the development of cold-atom sensors for inertial navigation by using laser cooling is illustrated in [10, 11], and a view of navigation applications by using atomic gyroscopes is discussed in [12]. Moreover, the challenges concerning the transport of matter–wave interferometers out of the laboratory are cited in [13].

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Accordingly, the nanostructures have been always seen as good candidates for working in semiconducting and sensor functions and their features were investigated in this regard in several works [14–16]. On one hand, some research papers reported the difficulties that can be encountered during the development of cold-atom sensors [17, 18]. On other hand, the new generation and future experiments of cold-atoms sensors are proposed while using the property of quantum interferometry and the technique of laser cooling [19, 20].

As a result of these research papers, the inertial navigation by using cold-atom sensors has acquired a higher performance and more efficiency compared to typical optical gyroscopes [21]. The improvements in inertial navigation are due to cold-atom wavelength uncertainty that is less than in optical technologies of Fiber Optics Gyroscopes (FOG) by ten orders of magnitude. In addition, owing to their low temperature, cold atoms can provide more precision, low-noise measurements and higher signal performance compared to optical inertial sensors [22]. Moreover, measuring gravity in satellites and aircraft has become more efficient due to the implementation of cold-atom gravimeter sensor in these devices [23, 24]. In fact, the group at Stanford University (SU) developed the first cold-atom gravimeter sensor based on sodium atom \( ^2 \text{Na} \) and a resolution of \( 3 \times 10^{-9} \)g within a real interrogation time of 1000s was achieved in the 1990s [25]. After some developments, SU group achieved a measurement resolution of \( 1 \times 10^{-9} \)g in 2001 and a resolution of \( 5 \times 10^{-11} \)g after twenty-seven hours of interrogation time was achieved by Humboldt University (HU) in 2013, as presented in [26]. These developments are still underway in order to obtain higher sensitivity in cold-atom gravimeters and a large dynamic range by applying the atom interferometry and the laser with low-phase noise. In fact, the researchers of Humboldt University built an ultra-high sensitivity gravimeter in 2013 whose sensitivity of the gravimeter sensor is reached \( 4.2 \mu \text{Gal/} \sqrt{\text{Hz}} \) [27]. Otherwise, various ICT devices such as satellite, GPS and quantum computers are based on oscillation clocks that should have a stable frequency to achieve high performances in their functions [28, 29]. For this purpose, the quartz clocks based on quartz oscillation have been replaced by atomic clocks to improve the efficiency and the performance of ICT devices [30]. Indeed, the time counter in atomic clocks is achieved by exploiting the energy difference between two stationary quantum states in an ultracold atom Rubidium or Cesium [28, 31]. Recently, the Deep Space Atomic Clock (DSAC) engineered on June 24, 2019 at the Kennedy Space Center in Florida has a high accuracy with an uncertainty of less than 10 ns every 10 days, which is equivalent to one second in each 10 million years [32]. These improvements in clock oscillation help to assure the synchronization between ICT devices, engineer accurate navigation systems in transportation tools and ensure the financial transactions and data transmission between clients in real-time.

The positive influences of cold atoms on the efficiency and accuracy of ICT devices and sensors gave them more importance in material physics laboratories [7]. Therefore, physicists have carried out various experiments and numerical analyses with cold atoms in different dimensional speckles. For this purpose, Anderson localization in one-dimensional (1D) for correlated random potentials is discussed in [33], and the propagation of cold atoms in two-dimensional (2D) speckle potentials is studied in [34, 35]. In addition, the analytical studies of localization of cold-atoms in 3D optical disordered speckles and numerical simulations of Elastic Scattering Time (EST) of matter waves in disordered potentials by using First-order Born Approximation (FBA) is reported in [36, 37]. However, the study of propagation of matter-wave by using FBA approximation for one diffuser leads to a significantly overestimates of scattering amount, a limited energy spectrum and it provides inefficient results on the metal–insulator transition in the disordered material nanostructures. For this reason, the FBA will be replaced by another approximation, which will be used to study the behaviour of cold atoms in optical speckles.

The main purpose of this paper is to investigate the diffusion and localization of cold atoms in 3D optical speckles for \( N \) diffusers created by an optical laser. In this numerical study, the SCBA approximation and spectral function are used to estimate the self-energy of matter-wave in speckles instead of FBA approximation. It is worth mentioning that the theoretical and numerical based simulations are among those useful tools for solving problems in the scientific topics [38–40]. Indeed, the 3D optical speckles considered in our study can be used to measure various dynamic properties relevant in medical diagnosis and to improve the medical imaging [41]. In addition, it can be useful to analyse the burn depths and we can apply it to monitor the various changes in blood sugar as part of the diabetes treatment. In this work, the SCBA approximation for \( N \) diffusers is performed to assess the diffusion and localization of cold-atoms in disordered potentials and to measure the diffusion time \( \tau \) and mean free path \( l \) between two diffusers. In addition, it is also used to show the effect of energy \( \varepsilon \) and correlation length \( \xi \) on the self-energy of matter waves. Otherwise, the spectral function is adopted to study the energy distribution evaluated in BECs and the effect of disorder amplitude \( V_0 \).

This paper is organised as follows: at the beginning, an introduction of cold atoms efficiency on ICT devices and sensors is provided, which synthesizes the main
contributions of this study. In the next part, an overview of laser cooling and cold atoms localization in optical speckles is illustrated. In addition, the SCBA approximation for the self-energy and the spectral function are detailed. Moreover, the numerical results of FBA and SCBA approximations for one and \( N \) diffusers, respectively, are discussed. Finally, the global conclusions of this study are presented and the numerical algorithm for the computation of the latter quantities by using “Simpson” method is clarified in the appendix.

2. An overview of laser cooling and cold atoms localization in optical speckles

The concept of laser cooling and cold atoms diffusion in optical speckle potentials has an importance in this study. For this purpose, an overview of the major advances in this field is given in the two following subsections.

2.1. An overview of laser cooling

In 1960, the American physicist Theodore Maiman invented the ruby laser [42]. After that, the inventor Peter Sorokin achieved the first liquid laser in 1966 [43]. Indeed, many experiments are performed to apply the laser in various fields of our daily life. For instance, lasers play a major role in CD, DVD and barcode readers. In addition, they are used widely in road information for obstacles detection and vehicles speed measurement [44]. On other hand, the development of the lasers has allowed spectral advances in quantum researches, such as quantum optics, atoms cooling and ultra-cold sensors [45, 46]. The high efficiency of optical lasers is due to their photon absorption property, which has been used in atoms cooling.

The research in ultra-cold atoms in laser fields has much developed over the past 30 years. For this focus, the physicists have carried out experiments with atoms under the action of laser beams to reach values of the temperatures in the range of a few hundred of nK. Indeed, the atoms cooling are typically performed by a single laser beam [47], which is used to control the atom motion. The latter depends mainly on the absorption and emission of photon waves when the atomic states shift from a ground level \( E_1 \) to another one \( E_2 \) and in the reverse process. However, in the presence of a single laser beam, the recoil velocity of atoms is very tiny, but if a large number of laser beams is placed in the right direction, the temperature will be reduced significantly and the atoms velocity will be decreased. For this purpose, the Doppler cooling technique has been applied since 1975 to improve the efficiency and cooling properties of atoms [48, 49]. This technique consists in placing the atoms between two laser beams, as shown in Fig. 1. In fact, the frequency \( f \) of two laser beams should be the same and precisely fixed at a value slightly lower than the atomic state frequency \( f_0 \) for absorption and emission of photons \((f<f_0)\). As a result of Doppler cooling, a frictional force \( F \) opposite to the atomic velocity \( V \) is obtained with: \( F = -aV \), where \( a \) represents the friction coefficient.

The technique of Doppler cooling can be generalised in 3D by using six laser beams and by creating an intangible trap, as illustrated in Fig. 2. The laser photons create a viscous medium in which the atoms will slow down and will be cooled. This trapped gas is often called optical molasses. Moreover, the advances in laser cooling and atoms trapping have made it possible to control the atoms by using new techniques, such as Magneto-Optical Traps (MOTs) and Magnetic Confinement (MC).

The principle of MOTs technique was proposed by the physicist Jean Dalibard [50]. This technique requires obtaining an optical molasses and a magnetic field gradient to improve the laser cooling efficiency [51]. In fact, the first atoms cooling by MOTs technique is achieved in 1987. In MOTs, the atoms are captured by a trap, which is made by three pairs of lasers and a magnetic field generated by two coils, as shown in Fig. 3. However, this technique does not allow achieving the BEC condensation. For this purpose, the MOTs technique is replaced by a purely magnetic trapping.

Magnetic Atoms Trapping (MAT) is based on the induction of a magnetic field in the opposite direction of the magnetic moment of the atoms [52]. In that platform, the atoms are attracted to areas of low magnetic field and a potential \( V(r) \) is obtained due to the interaction between the magnetic field and the total atomic spin. This potential \( V(r) \) can be defined as follows:

\[
\left\{
\begin{array}{l}
V(r) = -\mu |B(r)|, \\
\mu = g_F m_F \mu_B
\end{array}
\right.
\]

with \( \mu \) is the magnetic moment of atoms, \( m_F \) represents the hyperfine state, \( g_F \) denotes Landé g-factor and \( \mu_B \) is the Bohr magneton.

Since 1987, the MAT technique has been improved by introducing the evaporative cooling that eliminates the atoms which have high energy by using an atomic confining potential \( U \), as illustrated in Fig. 4. Indeed, the coldest atoms situated inside the potential have a

![Fig. 1 Doppler cooling technique](image-url)
temperature that is about 300 billion times lower than room temperature.

The development of different techniques of laser cooling, such as MOT, MAT and evaporative cooling technique, led to the achievement of the condensate of a rubidium $^8_7\text{Rb}$. In fact, Einstein predicted in 1924 this condensation phenomenon in 1925 and it was observed for the first time in 1995 by Cornell, Ketterle and Wieman in a dilute ultracold gas [53]. This experiment achievement of BEC condensate was rewarded by a Nobel Prize in physics in 2001 [54]. Indeed, the BEC condensate obtained is studied to achieve a temperature of boson particle waves $T$ lower than the temperature of the condensate $T_{\text{BEC}}(T << T_{\text{BEC}})$[55]. In this context, the thermal de Broglie wavelength $\lambda_{\text{dB}}$ accounts for the spatial extent of boson particles and can be used to measure interatomic distance $d \approx n^{1/3}$, in which the $n$ represents the spatial density of an atomic cloud. The phase-space density $D$ and

$$D = n\lambda_{\text{dB}}^3 \approx 1,$$

$$\lambda_{\text{dB}} = \sqrt{\frac{2\pi\hbar^2}{mk_B T}},$$

where $m$ indicates the atomic mass and $k_B$ represents the Boltzmann constant.

2.2. An overview of cold atoms localization in optical speckles

Anderson localization of ultracold atoms is performed in several groups and laboratories, such as the Institut d’Optique in Orsay [56]. The main purpose of these experiments is to study the matter-wave localization of a BEC condensate. In fact, these experimental results of matter-wave localization can be obtained in various dimensional geometries (1D, 2D and 3D). In One-Dimensional random potentials (1D), the cold atoms localization is directly observed and the wavelets generated by the scattering off the speckles interfere destructively in almost all the space [57]. In Two-Dimensional (2D) disordered potentials, since the localization length increases exponentially with energy, the unambiguous observation of localization has been achieved only very recently, in relatively large lattices [58]. In Three-Dimensional (3D) random potentials, the metal–insulator phase transition has also been observed [59]. To this end, matter-wave localization is reached by using a single and a superposition of plane waves in a disordered potential $V(z)$.

In the last mentioned experiment, a single plane wave has been first propagated in a disordered potential. This plane wave is characterized by a wave vector $k$ and by an energy that is equal to $E_k = \hbar^2 k^2/2m$, while the disordered potential is given by randomly distributed barriers of
average value $V_R$, and spatial variation length $\delta Z$. For this experiment, the spatial variation $\delta Z$ was set to be lower than the wave plane length $\lambda_k$, whereas the plane-wave energy $E_k$ was imposed to be smaller than random amplitude $V_R(E_k < \lambda V_R)$. Under these conditions, the plane-wave localization is achieved where the wave function decreases exponentially in the potential, as shown in Fig. 5. This spatial variation is described by localization length $L_{loc}(k)$ and is equal to the inverse of the Lyapunov exponent.

$$\gamma(k) = \frac{1}{L_{loc}(k)} = -\lim_{|z| \to \infty} \left< \frac{\log(r(z))}{|z|} \right>, \quad (3)$$

In a scattering experiment, a plane wave coming from infinity propagates on the trapped atoms for $k < k_c$. This incoming wave undergoes total reflection inside the medium, which decays exponentially from the boundary of optical speckles towards its interior. This exponential decay is not a sufficient criterion to obtain localization in the expansion of BEC, since it cannot assure the existence of states deep inside the optical speckles [60]. For this reason, plane wave superpositions are handled to achieve the expected objectives. As a result, the density of matter-wave $n(z)$ in one dimension is given by the superposition of localized wave functions $\phi_k(z)$, as presented in Eq. (4).

$$n(z) = \left< |\psi(z)|^2 \right> = 2 \int_0^\infty dk D(k) \left< |\phi_k(z)|^2 \right>, \quad (4)$$

where $\left< |\psi(z)|^2 \right>$ represents the average of random potentials and $D(k)$ is the density in the phase space.

The study of cold atoms localization in optical speckles begins with the description of the model of self-energy and of the spectral function, which is detailed in the next section.

3. SCBA approximation for the self-energy and spectral function

The study of diffusion and localization of cold atoms in 3D disordered potentials is related to various factors, such as the diffusion time and the mean free path between two diffusers. The properties of these quantities are related to the approach used to estimate the self-energy [62]. In the present study, the latter quantity, as well as the spectral function, will be computed in the SCBA approximation.

The SCBA approximation will be developed by starting from Green’s functions and Dyson equation [61, 62]. Indeed, Schrödinger equation is used to define the Green’s functions and to subsequently introduce the Dyson equation.

3.1. Green’s functions

At each site in optical speckles, the disordered potential is generated by properly convoluting a correlated sequence to reproduce the potential distribution and the correlation function defined in Eqs. (5) and (6), respectively [63].

$$P(V) = \Theta(V + V_0) \exp(-\frac{V}{V_0}), \quad (5)$$

with $\Theta$ is the Heaviside function and the disorder amplitude $V_0$ is related to the disorder variance $U$ by $U = V_0^2$.

The correlation function of the random potential is:

$$\langle V(r') V(r') \rangle = V_0^2 C(r/\xi), \quad (6)$$

where $C(r/\xi) = (\sin(r/\xi)/(r/\xi))^2$ and $\xi$ is the correlation length.

Conceptually, the Schrödinger equation associated with the Hamiltonian can be defined as follows:

$$\hbar \frac{\partial \psi}{\partial t} = H\psi = (H_0 + V)\psi, $$

where $H_0 = -(\hbar^2/2m)\nabla^2$ represents the disordered potentials and $\psi$ symbolizes the wave function.

The state $\psi(t)$ at time $t$ is given by the application of evolution operator $U(t, t_0)$ on the state $\psi(t_0)$:

$$\left\{ \begin{array}{l}
|\psi(t)\rangle = U(t, t_0) |\psi(t_0)\rangle \\
\quad = e^{-\frac{i}{\hbar}(t-t_0)/\hbar} |\psi(t_0)\rangle
\end{array} \right. ,$$

(8)

Moreover, the spatial behaviour of the state at time $t$ can be obtained by projecting Eq. (8) on the position representation $r$. 

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Fig. 5 Anderson localization of cold atoms in optical speckles

---
\[ \langle r | \psi(r) \rangle = \left\langle r | e^{-i \frac{H}{\hbar} t} \psi(t_0) \right\rangle, \]  

(9)

By plugging the completeness relation into Eq. (9), the state in configuration picture \( \langle r | \psi(t) \rangle \) becomes:

\[
\begin{aligned}
1 &= \int dr_i \langle r_i | \langle \psi(r) \rangle \\
\langle \psi(t) \rangle &= \int dr_i \langle r_i | e^{-i \frac{H(r-t_0)}{\hbar}} \langle r_i | \psi(t_0) \rangle.
\end{aligned}
\]

(10)

The Green’s functions can be thus defined as follows:

\[
G(r_i, r, t) = \langle r_i | e^{-i \frac{H(r-t_0)}{\hbar}} | r \rangle = \sum_n \varphi_n^*(r_i) \varphi_n(r) e^{-i \epsilon_n (r-t_0)},
\]

(11)

where \( \epsilon_n \) and \( \varphi_n \) represent eigenvalues and eigenvectors, respectively, of Hamiltonian operator \( H \).

### 3.2. Dyson equation

In this section, Dyson equation will be introduced based on the Green’s functions in Eq. (11). By applying a Fourier Transform (FT) on Eq. (11), one obtains:

\[
G(r_i, r, \epsilon) = \int_{-\infty}^{+\infty} dt e^{i \epsilon t/\hbar} G(r_i, r, t),
\]

(12)

By performing the integral of Eq. (12) and by including the imaginary part to energy \( (\epsilon \pm i \delta) \), Green’s equation result is simplified as follows:

\[
G_e(r_i, r, \epsilon) = \frac{\varphi^*(r_i) \varphi(r)}{\epsilon - \epsilon_n \pm i \delta}.
\]

(13)

The result obtained in Eq. (13) can be used to define the Green’s operators \( \hat{G} \) and \( \hat{G}_0 \) associated to Hamiltonians \( H \) and \( H_0 \), respectively:

\[
\begin{aligned}
\hat{G}(\epsilon) &= \frac{1}{\epsilon - H \pm i \delta}, \\
\hat{G}_0 &= \frac{1}{\epsilon - H_0 \pm i \delta}.
\end{aligned}
\]

(14)

Schrödinger equation defined in Eq. (7) can be rewritten using the relation between \( G \) and \( \hat{G}_0 \). Therefore, the Dyson equation is obtained by multiplying the first relation of Eq. (14) by \( \hat{G}_0 \), and by using the second one \( (\epsilon \pm H_0) \hat{G}_0 = 1 \) and reads:

\[
\hat{G} = \hat{G}_0 + \hat{G}_0 V \hat{G},
\]

(15)

Indeed, Eq. (15) is considered as iterative development of self-energy \( \Sigma \). By using this equation, the diffusion operator \( \hat{i} \) is introduced.

\[
\hat{i} = \hat{V} + i \hat{G} \hat{V},
\]

(16)

In fact, Eq. (16) represents the diffusion operator for one diffuser that is used in FBA approximation. In the SCBA approximation the RHS of Eq. (15) is expanded in powers of \( V \hat{G} \), using \( V \hat{G} = V \hat{G}_0 + V \hat{G}_0 \hat{G}_0 + \cdots \), whereas by combining Eqs. (15) and (16) one gets \( G = \hat{G}_0 + \hat{G}_0 V \hat{G}_0 + \cdots \). Plugging the expansion into the latter equation and labelling with \( \hat{i} \) each of the \( N \) diffusers, one obtains:

\[
\hat{i}(r, \hat{r}) = \hat{V}_i + \hat{V}_i \hat{G}_0 \hat{V}_i + \hat{V}_i \hat{G}_0 \hat{V}_i \hat{G}_0 \hat{V}_i + \hat{V}_i \hat{G}_0 \hat{V}_i \hat{G}_0 \hat{V}_i \hat{G}_0 \hat{V}_i \cdots,
\]

(17)

The operator \( \hat{i} \) refers to the scattering off a particle centred in \( R_i \) and is related with operator \( \hat{i} \) by the following equality:

\[
\hat{i}(r, \hat{r}) = tr - R_i, \hat{r} - R_i.
\]

(18)

Finally, the Dyson equation for \( N \) diffusers can be defined as:

\[
\hat{i} = \sum_{i}^{N} \hat{i}_i + \sum_{i \neq j}^{NN} \hat{i}_i \hat{G}_0 \hat{j}_i + \sum_{i \neq j \neq k}^{NNN} \hat{i}_i \hat{G}_0 \hat{j}_i \hat{G}_0 \hat{k}_i + \cdots,
\]

(19)

In Eq. (19), the first sum refers to simple diffusion, while the second and third represent the double and triple diffusions between the incident wave and the observation point, respectively.

### 3.3. SCBA approximation model

Analytically, the self-energy \( \Sigma \) is related to the average of Dyson equation, which can be calculated by the average of Green’s functions [64]. For this purpose, the average of Dyson equation (\( \langle \hat{i} \rangle \)) and Green’s functions (\( \langle \hat{G} \rangle \)) are given by the equations:

\[
\begin{aligned}
\langle \hat{G} \rangle &= \hat{G}_0 + \hat{G}_0 \sum \hat{G}_0 + \hat{G}_0 \sum \hat{G}_0 + \hat{G}_0 \sum \hat{G}_0 + \cdots \\
\langle \hat{i} \rangle &= \sum + \sum \hat{G}_0 \sum + \sum \hat{G}_0 \sum \hat{G}_0 \sum + \cdots
\end{aligned}
\]

(20)

Indeed, the self-energy \( \Sigma \) represents the sum of diffusers that can be expressed by blue circles, as illustrated in Fig. 6. The half dotted circles indicate that the diffusers are correlated by a correlation function, while the half rectangle represents the recurring diffusion.

Much of the analytical study of diffusion and localization of matter-wave in 3D disordered potentials that will follow depends on the approximation of the self-energy \( \Sigma(\epsilon, k) \) [65], which is a complex function. The relation between the Green’s functions \( G(\epsilon, k) \) and the former quantity is given by:
The SCBA approximation will be developed by using the Green’s and structure functions \((G(\epsilon,k), U(k-k'))\), as:

\[
\sum (\epsilon, k) = \sum_k U(k-k')G(\epsilon,k),
\]

where the complex Green’s function \(G(\epsilon,k')\) is given by:

\[
G(\epsilon,k') = \frac{1}{\epsilon - (\hbar^2 k'^2/2m) - \sum(\epsilon,k')},
\]

In addition, the structure functions \(U(k-k')\) and the operator \(\sum_{k'}\) are defined as follows:

\[
\begin{cases}
\sum_{k'} = \int \frac{d^3k'}{(2\pi)^3} \\
U(k-k') = U \sum_{k'} \left( \frac{\sin(x/\xi)}{(x/\xi)} \right)^2 e^{i(\vec{k}-\vec{k'}) \cdot \vec{x}}
\end{cases}
\tag{24}
\]

Using the relation in Eq. (24), the self-energy in SCBA approximation in 3D thus contains a Fourier Transform (FT):

\[
\sum(\epsilon, k) = \frac{4\pi U}{(2\pi)^3} \int \frac{d^3k}{(2\pi)^3} \int \frac{d^3x}{(2\pi)^3} \left( \frac{\sin(x/\xi)}{(x/\xi)} \right)^2 e^{i(\vec{k}-\vec{k'}) \cdot \vec{x}} G(\epsilon,k),
\tag{25}
\]

By adopting spherical coordinates and integrating over the angular variable, Eq. (25) takes the form:

\[
\sum(\epsilon, k) = \frac{2\pi U}{(2\pi)^3} \int_0^\infty \frac{dk'}{k'} \int_0^\infty \frac{dx}{x} \sin^2 \left( \frac{x}{\xi} \right) \\
\times \sin \left( \frac{kx}{k'} \right) \sin \left( \frac{k'x}{k} \right) G(\epsilon,k),
\tag{26}
\]

Finally, the self-energy in the SCBA approximation depends essentially on three parameters; the matter-wave number \(k\), the diffusers wave number \(k'\) and the correlation length \(\xi\);

\[
\sum(\epsilon, k) = \frac{2\pi U}{\pi} \int_0^\infty \frac{dk'}{k'} \int_0^\infty \frac{dx}{x} \frac{I(k,k')}{\sqrt{\epsilon - \xi k - \sum(\epsilon,k')}},
\tag{27}
\]

where \(\epsilon = \frac{\hbar^2 k^2}{2m}\) and \(I(k,k')\) is the new structure function, which is given by:

\[
I(k,k') = \frac{-\pi}{16k^2} \left[ \frac{2}{\xi} - k - k' \right] + 2|k - k'| - \frac{k - k'}{\xi} - \left| k - k' - \frac{2}{\xi} \right| + \left| k' + k - \frac{2}{\xi} \right|,
\tag{28}
\]

In addition, the diffusion time \(\tau\) and the mean free path between two diffusers \(l\) can be calculated by using the imaginary part of the self-energy in SCBA approximation [62]:

\[
\tau = \frac{\hbar}{2\text{Im}(\sum(\epsilon,k))}, \\
l = \frac{\hbar^2 k_0}{2m \text{Im}(\sum(\epsilon,k))},
\tag{29}
\]

where \(k_0 = \frac{\sqrt{2m \epsilon_0}}{\hbar} = \frac{1}{\xi}\)

### 3.4. Spectral function model

The modelling of spectral function \(A(\epsilon,k)\), which represents the energy distribution of a plane wave of wavevector \(k[66, 67]\), allows studying various parameters linked to the matter-wave diffusion in 3D disordered potentials, such as the diffusion time \(\tau\) and the mean free path between two diffusers \(l\). This function can be defined starting from the complex Green’s function \(G(\epsilon,k)\) as follows:

\[
A(\epsilon,k) = -\frac{1}{\pi} G(\epsilon,k),
\tag{30}
\]

On one hand, the spectral function can be also described by using the imaginary part of self-energy in the SCBA approximation, as:

\[
A(\epsilon,k) = \frac{1}{\pi} \frac{-\text{Im}(\sum(\epsilon,k))}{\sqrt{\epsilon - k^2 - \sum(\epsilon,k)^2}},
\tag{31}
\]

### 4. Results and discussion

Numerical simulations are performed for the self-energy in the FBA, SCBA approximations and the spectral function models. The model of FBA approximation for one diffuser is presented in Refs. [42, 43] and the algorithm, whose scheme is illustrated in the appendix, is used to achieve the required results. The experimental parameters of diffusion and localization of matter-wave in 1D disordered potentials, which have been used in the laboratory of Orsay [56] are chosen as numerical parameters in this simulation.
4.1. Results of FBA and SCBA approximations

Firstly, the FBA and SCBA approximations are tested at constant energy \( e \) by varying the values of wave number \( k \). In the numerical solutions, the energies of SCBA model for \( N \) diffusers are expressed in energy scale units \( \varepsilon_n \), while the number \( k \) is expressed in units \( 1/\xi \) and indicated as \( k_\xi \). In particular, for the simulations related to Figs. 7 and 8, the parameters are defined in Table 1 as follows:

Figures 7 and 8 represent the energy displacement \( \varepsilon_k \) and cold atoms diffusion in FBA and SCBA approximation for one and \( N \) diffusers, respectively, in optical speckles. Indeed, the results of energy displacement \( \varepsilon_k \) are obtained by computing the real part of the self-energy in FBA and SCBA approximations, while the cold atoms diffusion is studied by considering the imaginary of both models. As a result, the energy displacement \( \varepsilon_k \) decreases for \( k_\xi \leq 1 \) and, whereas the opposite trend is observed for \( (k_\xi \geq 1) \). This change in the behavior of energy as a function of the wave-number signals the emergence of a midgap state that occurs at the band edge of the spectrum [68]. In addition, the convergence of energy displacement towards zero value is ensured for high wave numbers, for both FBA and SCBA approximations, as shown in Fig. 7. This convergence is obtained when the wave number is close to 10 \( (k_\xi \approx 10) \) where the motion of cold atoms is less affected by the impurities. According to Fig. 7, the upper band edge of the spectrum and the displacement in energy generated by \( N \) diffusers are lower than for one diffuser. These results can be useful for improving the nanostructure in cold-atom sensors by decreasing the conductivity and reducing the energy consumption. On the other hand, the cold atoms diffusion in FBA and SCBA approximations for one and \( N \) diffusers vanishes for \( k_\xi > 3 \), as illustrated in Fig. 8. For \( k_\xi \leq 1 \), the curve obtained in FBA approximation is constant, while it decreases slowly for rising wave-number in SCBA approximation. Therefore, the cold atoms in 3D optical speckles remain at the initial diffusive state for FBA approximation, without any scattering of matter waves in disordered potential. This result obtained for \( k_\xi < = 1 \) is due to the fact that the probability of encountering the cold-atoms with one diffuser is very small compared to the case of \( N \) diffusers. For \( k_\xi > = 1 \), the cold atoms diffusion decreases exponentially towards zero value. Indeed, cold atom diffusion is halted at wave number equal or greater than 3 \( (k_\xi \geq 3) \) that means that the cold atoms in 3D disordered potentials is localized. According to Fig. 7, the SCBA approximation curve lies below FBA approximation curve by a factor equal to 1.66. This result obtained in numerical simulation of imaginary part suggests that the relaxation time of cold atoms diffusion in optical speckles for \( N \) diffusers is higher than for one diffuser.

Secondly, the effect of length correlation \( \xi \) and matter waves energy \( \varepsilon \) on the self-energy is illustrated by analysing the real and imaginary parts of SCBA approximation. Indeed, the numerical simulation of length correlation effect is tested at \( \xi = 0.6, \xi = 0.8 \) and \( \xi = 1 \), while the matter waves energy effect is studied at \( \varepsilon = 0.6 \varepsilon_\xi, \varepsilon = 0.8 \varepsilon_\xi \) and \( \varepsilon = 1 \varepsilon_\xi \).

Figures 9 and 10 represent the effect of correlation length \( \xi \) on the self-energy. According to Fig. 9, as the correlation length increases, then the energy displacement and upper band edge are reduced. In addition, the response time of cold atoms stabilization decreases accordingly. Therefore, the increase in correlation length can give rise to a lessening of the disordered material conductivity.

![Fig. 7 Energy displacement in FBA and SCBA for one and diffusers, respectively, in 3D optical speckles](image)

![Fig. 8 Imaginary part of the self-energy in FBA and SCBA for one and diffusers, respectively, in 3D optical speckles](image)

![Table 1 Parameters values of first simulation](image)
increasing the recoil velocity of atoms and reducing the energy consumption. The cold atoms diffusion and localization are thus related to the values of correlation length $\xi$, as illustrated in Fig. 10. Indeed, the diffusion in disordered potentials is slowed and the cold atoms become eventually strongly localized when the correlation length is increased. For this numerical simulation, the cold atoms are localized for $k_\xi = \frac{3}{\xi}$ and for $\xi = 1 \mu m$.

The effect of matter-wave energy $\varepsilon$ on the self-energy is illustrated in Figs. 11 and 12. Indeed, the variation of matter-wave energy can affect the energy displacement $\text{Re} \left( \sum (\varepsilon, k) \right)$ only at low momenta $k_\xi < 1.6/\xi$, as shown in Fig. 11. Interestingly, the increase in matter-wave energy can lead to a rise in the disordered material conductivity, as explained in [69, 70]. Otherwise, when the matter-wave energy $\varepsilon$ decreases, then the time response of localization increases and the wave number $k_\xi$ required for matter-wave localization in 3D disordered potentials diminishes, as illustrated in Fig. 12 This result obtained in imaginary part of SCBA approximation is justified by the behaviour of both the mean free path $l$ and the diffusion time $\tau$. According to Figs. 13 and 14, both the mean free path and the diffusion time exhibit a decreased when the matter-wave energy is increased, which means that the atoms are still dispersed and the matter-wave localization is not achieved.
In third simulation, the FBA and SCBA approximation models are tested by varying the energy distribution $e$ at wave number equal to zero ($k_n = 0$). This numerical simulation is handled for amplitude $V_0$ and correlation length $\xi$ equal to one in our units ($V_0 = 1 \, e_\xi$; $\xi = 1 \, \mu m$). Figures 15 and 16 represent the energy displacement $e_k$ and cold atoms diffusion in FBA and SCBA approximation in terms of energy distribution $e$ at $k_n = 0$. Indeed, the energy displacement $\text{Re} (\sum(e, k))$ decreases significantly when the energy is negative ($e < 0 \, e_\xi$) or higher or equal to four ($e \geq 4 \, e_\xi$), whereas it is increased exponentially for energy bounded between 0 and 4 ($e \in [0, 4]$). The maximum values of the energy displacement are reached for $e = 0 \, e_\xi$ and $e = 4 \, e_\xi$, as shown in Fig. 15. In fact, the convergence of energy displacement towards zero value is achieved, which means that the scattering of matter waves in disordered potential is very tiny. According to Figs. 15 and 16, the lower band edge of the spectrum and the energy displacement in SCBA approximation are smaller than in FBA approximation. This result is in agreement with the one obtained in Fig. 7. Therefore, by tuning the wave number $k_\xi$ and energy distribution in 3D disordered potentials with $N$ diffusers one can improve the characteristics of cold atom-based sensors by increasing the localisation time and reducing the energy consumption. Otherwise, the nonzero values of cold atoms diffusion in FBA and SCBA approximations are found only when the energy is confined between 0 and 4 ($e \in [0, 4]$) and the cold atoms localization is achieved at $e = 4 \, e_\xi$ according to both approximations, as illustrated in Fig. 16. However, the localization time in SCBA approximation is faster than FBA approximation, which has been justified by studying the difference in mean free path and diffusion time in FBA and SCBA approximations. Indeed, the curves of mean free path and diffusion time lie over the curve of FBA approximation, as shown in Figs. 17 and 18, pointing out that the atoms are less dispersed and can be more rapidly localized in SCBA than FBA approximation.

According to the results obtained in our numerical simulations, the application of the SCBA approximation in 3D disordered potentials instead of the FBA approximation gives rise to the following differences:
• The curve of imaginary part of SCBA lies below the curve of the FBA approximation. Therefore, the time response of cold atoms localization in SCBA approximation is smaller than in FBA approximation.

• The probability of encountering the cold-atoms with one diffuser is very small compared to \( N \) diffusers. Therefore, the cold atoms can be localized rapidly in SCBA compared to the FBA approximation.

• The SCBA can be useful for modelling the materials exploitable for sensors based on cold atoms.

• In the beginning of localization, the atoms are less scattered in FBA and SCBA approximation.

• The energy displacement in SCBA is lower than in the FBA approximation.

4.2. Results of spectral function

The spectral function \( A(\varepsilon, k) \) can be analysed to study the diffusion and localization of cold atoms in 3D optical speckles, since it allows knowing the number of atoms that are diffused in the disordered potential. Here, the numerical simulation of spectral function is evaluated for variable wave number \( k_\xi \) at different values of matter-wave energy \( \varepsilon \) and disorder amplitude \( V_0 \).

Figure 19 represents the behaviour of the spectral function as a function of the matter-wave number for \( \varepsilon = 0.5\varepsilon_\xi, \varepsilon = 1\varepsilon_\xi, \varepsilon = 2\varepsilon_\xi \) and \( \varepsilon = 3\varepsilon_\xi \) at a disorder variance equal to \( 1\varepsilon_\xi^2 \) \((U = 1\varepsilon_\xi^2)\). In this result, the numbers of atoms that will be diffused in 3D disordered potentials is increased when the matter-wave energy increased. It is significantly observed in Fig. 19 that the spectral function curve at \( \varepsilon = 3\varepsilon_\xi \) takes the forms of BEC condensation curve (Lorentzian broadening) [36, 71], which means that the cold atoms are at the beginning of localization process. In fact, the results obtained in Fig. 19 confirmed the curve achieved in Fig. 12 that means that the cold atoms localization become strongly localized whenever the matter-wave energy is small.

Figure 20 represents the variation of spectral function in terms of matter-wave number for \( U = 0.5\varepsilon_\xi^2, U = 1\varepsilon_\xi^2 \) and \( U = 2\varepsilon_\xi^2 \) at matter-wave energy equal to \( 3\varepsilon_\xi \) \((\varepsilon = 3\varepsilon_\xi)\). In this figure, the amplitude of spectral function is plotted for variable disorder variance \( U \). It is shown that an increase in the last-mentioned quantity leads to a decrease in the number of atoms that will be diffused. At the same time, the fraction of localized atoms increases.

5. Conclusions

The accuracy of sensors installed in industrial, electrical and ICT equipment are getting increasingly important in their functions. For this purpose, much of the current research focuses on the improvement of the cold atom sensors, such as atomic clocks, gravimeters and gyroscopes. In addition, the most recent experimental works make use of laser cooling to achieve BEC condensation.
and aim to study the scattering of cold atoms in 1D, 2D and 3D optical speckles.

In this paper, the analytical and numerical study of diffusion and localization of cold atoms in 3D optical speckles is carried out. In fact, the numerical analysis involves the computation of the self-energy in the FBA and SCBA approximations, as well as the spectral function by using an algorithm developed by using Fortran language. The numerical results show that the SCBA approximation can be useful to improve the disordered material of cold atoms sensors by increasing the time response of matter waves localization. The results obtained in this study are justified by examining both the diffusion time and the mean free path as functions of the matter-wave energy.

The study of cold atoms localization in 3D optical speckles can allow improving the analysis tools and imaging for medical diagnosis, including the measurement of burn depths and blood sugar.

**Appendix: numerical computation of the self-energy**

The models of SCBA approximation and spectral function require performing the functional integration in Eq. (27), which is performed by using the “Simpson” rule in a code written in the language “Fortran 90”, as detailed in Fig. 21. Indeed, the value of $\sum (e, k')$ is given by $-i\alpha$ and the complex function of Eq. (27) is separated into the real and the imaginary parts.

$$
\begin{align*}
\text{Re} \left( \sum (e, k) \right) &= \frac{2 U \xi^2}{\pi} \int_0^\infty dk' \text{Re} F_s (e, k, k') \\
&= \frac{2 U \xi^2}{\pi} \int_0^\infty dk' k'^2 I(k, k') \frac{(e - \epsilon_k)}{(e - \epsilon_k)^2 + \alpha^2} \\
\text{Im} \left( \sum (e, k) \right) &= \frac{2 U \xi^2}{\pi} \int_0^\infty dk' \text{Im} F_s (e, k, k') \\
&= \frac{2 U \xi^2}{\pi} \int_0^\infty dk' k'^2 \frac{-I(k, k') \alpha}{(e - \epsilon_k)^2 + \alpha^2}
\end{align*}
$$

(32)

On the other hand, the function integration is performed by a sampling frequency $f_s$ of 1 MHz. For this analytical study, the real part “$\text{Re} \left( \sum (e, k) \right)$” is handled to evaluate the energy displacement $\epsilon_k$, while the imaginary part in

![Fig. 21 Functional integration algorithm for the computation of the real and the imaginary parts of the self-energy](image-url)
SCBA approximation \( \text{Im} \left( \sum (a, k) \right) \) is calculated to study the cold atoms diffusion.

The integrations in the RHS of Eq. (32) are performed in a bounded interval \([a, b]\), as announced, by making use of the following Simpson method:

\[
\int_0^\infty dk' F_k(k, k') = \left( \frac{b - a}{n} \right) \left( S_a + 2S_{\text{even}} + 4S_{\text{odd}} + S_b \right)
\]

(33)

where \( \frac{(b - a)}{n} \) represent the sampling time \( T_s \). In addition, \( S_a \) and \( S_b \) denote the values of real and imaginary parts of the self-energy in the SCBA approximation at the interval boundaries \( a \) and \( b \), respectively. Moreover, \( S_{\text{even}} \) and \( S_{\text{odd}} \) represent the sum of \( \text{Im} \_F_k \) and function when the values of sampling time \( T_s \) is even and odd, respectively. The value of \( S_{\text{even}} \) and \( S_{\text{odd}} \) can be given by the global equation below:

\[
S_{\text{even}} = \sum_{m=1}^{n/2-1} F_k(k, k') \quad \text{for } j = 2m, \ m \in N \setminus \{0\}
\]

(34)

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Declarations

Conflict of interest In this study, all authors have no conflict of interest to declare.

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