Interplay between the repulsive and attractive interaction and the spatial dimensionality of an excess electron in a simple fluid

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Abstract

The behavior of an excess electron in a one, two and three dimensional classical liquid has been studied with the aid of Chandler, Singh and Richardson (CSR) theory [J. Chem. Phys. 81 1975 (1984)]. The size or dispersion of the wavepacket associated with the solvated electron is very sensitive to the interaction between the electron and fluid atoms, and exhibits complicated behavior in its density dependence. The behavior is interpreted in terms of an interplay among four causes: the excluded volume effect due to solvent, the pair attractive interaction between the electron and a solvent atom, the thermal wavelength of the electron ($\lambda_e$), a balance of the attractive interactions from different solvent atoms and the range of repulsive interaction between electron and solvent atom. Electron self-trapping behavior in all the dimensions has been studied for the same solvent-solvent and electron-solvent interaction potential and the results are presented for the same parameter in every dimension to show the comparison between the various dimensions.
I. INTRODUCTION

The behavior of an excess electron in a wide variety of fluids has been an interesting topic for many years. In the gas phase or the dilute liquid phase, the electron behaves almost like a free particle. As the solvent density increases, the electron exhibits different properties depending upon the nature of the solvent and electron-solvent interactions. At liquid density, the electron may become self-trapped in a cavity of solvent particles or remain quasifree depending upon the nature of electron-solvent interaction. Observed properties such as the electron mobility and the absorption spectra probe the nature of the electronic states in the fluid and phenomena of localization.

There are a broad range of problems in condensed matter physics that are intimately related to the problem of excess electrons in deformable medium. These include charge transfer kinetics in biological reactions, metal-insulator transitions in fluids, polarons, phonon-assisted hopping of charge carriers in semiconductors and insulators, quantum-tunneling, etc. While the excess electron problem belongs to the general problem of electrons in disordered materials, the liquid environment is in many ways different from the solid medium. In liquids, the constituent particles can diffuse, and local environment around the solute electron can be substantially different from that in solid.

When an electron is solvated in a polar liquid such as water or ammonia, the strong anisotropic electron-solvent interaction causes significant local modification of the equilibrium fluid structure. The electron becomes localized in a small cavity because molecules in a solvation shell orient to create a potential minimum. Even simple fluids are found to exhibit electron mobilities that change by many orders of magnitude as the density of the fluid is altered slightly. In super critical helium, for example, the electron mobility drops by over 4 orders of magnitude as fluid density increased by a factor of 2 in low density regime. The reason for this behavior is strong repulsion between electron and solvent atom. This causes the the depletion of the solvent atoms from the region of the electron and forms a highly localized state of the electron.

In many other nonpolar fluids such as Ar, CH4, etc. the electron always remains in a state of high mobility comparable to many semiconducting materials. An interesting density dependence of the mobility has been observed in them. It shows a minimum near critical fluid density and a maximum at liquid density.
Electronic states in reduced dimension are of considerable interest. For example, for a system less than two spatial dimension, electrons are localized with an infinitesimal amount of disorder. The interest in problems of electron or phonon propagation in a one dimensional random potential stems from the discovery and extensive experimental study of a certain class of organic or metallo-organic materials. These materials exhibit strongly anisotropic, quasi-one-dimensional behavior attributed to the fact that they consist of long chains, weakly interacting with each other. In many of these, the presence of a random potential has been proposed in order to explain their behavior. Electronic surface states play an important role in a wide variety of physical problems. For example, surface electrons on liquid helium has shown many interesting properties and led to important theoretical advances such as the spectrum of bound electronic states, electron transport on the He surface, effects due to deformation of the He surface, and the possibility that the electrons may form a two-dimensional crystal in the field of low-dimensionality physics.

The theory for the excess electrons in fluids developed by Chandler, Singh, and Richardson (CSR) is based on the path integral formulation of quantum theory which maps the behavior of the electron on to that of a classical isomorphic polymer. The solvent-induced potential surface for the self-interaction of the isomorphic polymer is evaluated using an integral equation (e.g., reference interaction site model). With known potential surface, the polymer statistics is solved using variational approach that allows the determination of electronic properties and the structure of the liquid near the electron. The input of the theory is the pure solvent structure factor and the electron-solvent particle interaction potential. The CSR theory in its formulation is applicable to an adiabatic solvent (i.e., solvent particles are treated classically), but has been extended to treat the effect of the quantum mechanical charge density fluctuation in the solvent particles. The calculated electron-absorption line shape and mobility are in good agreement with the simulations and experiments. The predictions of CSR theory were verified by computer simulations.

For a one-dimensional system we have shown recently that the repulsive and attractive parts of electron-solvent interaction potential lead separately to localization of electron, respectively, by creating cavity or forming a cluster of the fluids atoms around it. In two dimensional system we have shown that dispersion of the wavepacket associated with the solvated electron is very sensitive to the interaction between the electron and the fluid atoms, and exhibits complicated behavior in its density dependence. CSR theory has been extended
to calculate the effective mass as well as the density matrix of the excess electron in fluid.

The CSR theory involves three or more characteristic lengths, depending upon the nature of electron-solvent interaction. These lengths are the thermal wavelength of excess electron \( \lambda_e = \left( \beta \hbar^2 / m \right)^{1/2} \) (where \( \beta \) is the inverse of temperature in the unit of the Boltzmann constant \( k_B \), \( m \) is the mass of a bare electron, and \( \hbar \) is the Planck’s constant divided by \( 2\pi \)), characteristic length associated with the electron-solvent pseudopotential, and a length associated with the mean volume occupied by each solvent atom, which is related to \( \rho^* \beta \), where \( \rho^* = \rho_s \sigma^D \), \( \rho_s \) being the number density of the solvent and \( \sigma \) is the diameter of the solvent atom, and \( D \) is the spatial dimensionality of the system. The behavior of the excess electron is expected to depend sensitively on these lengths. Laria and Chandler have attempted to explain the contrasting behaviors of the electron in super critical helium and xenon on the basis of different ranges of the electron-solvent repulsive interactions.

In the present work we examine in detail the role played by different lengths and the spatial dimensionality of the system (in which we have considered the same solvent-solvent and electron-solvent model potential) to study the self-trapping behavior of the electron. The organization of the rest of the paper is as follows. In Sec. II we briefly review the CSR theory. In Sec. III we have presented the results and their discussions. Finally, Section IV presents concluding remarks. Appendix A provide some mathematical material for \( D \)-dimensional integration.

II. THEORY

The system we consider is a single electron dissolved in a single component classical solvent. In the CSR theory, an excess electron is mapped, using a discretized version of the path integral formulation of quantum mechanics, onto a polymer of \( P \) interaction sites or beads. Under this isomorphism, the electron can be viewed as a classical ring polymer.

The total potential energy can be written as

\[
U = U_{es}(r, \{R_i\}) + U_{ss}(\{R_i\})
\]

with

\[
U_{ss}(\{R_i\}) = \sum_{i>j=1}^N u_{ss}(|R_i - R_j|),
\]

where

\[
\lambda_e = \left( \beta \hbar^2 / m \right)^{1/2},
\]

\[
\rho^* = \rho_s \sigma^D,
\]

\[
D = \text{spatial dimensionality of the system}.
\]
and
\[ U_{es}(\mathbf{r}, \{\mathbf{R}_i\}) = \sum_{i=1}^{N} u_{es}(|\mathbf{r} - \mathbf{R}_i|) \] (3)

Here, \( \mathbf{r} \) denotes the position of the excess electron, \( \mathbf{R}_i \) is the collection of the coordinates for a solvent atom, and \( N \) is the number of solvent atoms and \( u_{es}(r) \) and \( u_{ss}(r) \) are, respectively, electron-solvent atom and solvent atom-solvent atom interaction potential. We consider a \( D \)-dimensional system of spheres of diameter \( \sigma \) in which the pair interaction between the solvent atoms is taken to be
\[ u_{ss}(|\mathbf{r}|) = \begin{cases} \infty & \text{for } |\mathbf{r}| \leq \sigma; \\ 0 & \text{for } |\mathbf{r}| > \sigma. \end{cases} \] (4)

where \( |\mathbf{r}| \) is the \( D \)-dimensional distance (for notational convenience the \( D \) dependence will not always be explicitly indicated). The electron-solvent atom interaction in a real system consists of a strong repulsion at short distance due to orthogonality requirements between wavefunctions of core electrons in the solvent particle and that of the excess electron and attraction at large distances due to dispersion interaction. However, in a system of neutral atoms the electronic states are determined primarily by the short range repulsive interaction or excluded-volume effect. The attractive interaction becomes important only at low densities. The interaction between the electron and solvent atom is taken to be
\[ u_{es}(|\mathbf{r}|) = \begin{cases} \infty & \text{for } r \leq d; \\ -\frac{\exp(-ar)}{ar} & \text{for } r > d. \end{cases} \] (5)

Here, \( d \) is the distance of closest approach between electron and solvent atom.

In CSR theory\(^4\) the partition function \( Z \) for an electron in a bath of classical particles is written as the functional integral
\[ Z = \int Dr(u) \int d\{\mathbf{R}_i\} \exp \left[ -\frac{1}{\hbar} \int_0^{\beta\hbar} du \left( \frac{1}{2} m |\dot{\mathbf{r}}(u)|^2 + U_{es}(\mathbf{r}, \{\mathbf{R}_i\}) \right) - \beta U_{ss}(\mathbf{R}_i) \right] \] (6)

where \( \mathbf{r}(u) \) is the electronic path in imaginary time which is periodic in time interval \( 0 \leq u \leq \beta\hbar \), i.e., \( \mathbf{r}(0) = \mathbf{r}(\beta\hbar) \). To concentrate our attention on the electron degrees of freedom, the partition function given by Eq.(6) can be written as
\[ Z = Z_s \int Dr(u) \exp \left\{ -\beta S_0[\mathbf{r}(u)] - \beta \Delta \mu[\mathbf{r}(u)] \right\} \] (7)

where \( Z_s \) denotes the partition function of the solvent, \( \Delta \mu[\mathbf{r}(u)] \) is the excess chemical potential for the fixed electronic path,
\[ \text{with, } \beta S_0[\mathbf{r}(u)] = \frac{1}{\hbar} \int_0^{\beta\hbar} du \frac{1}{2} m |\dot{\mathbf{r}}(u)|^2 \] (8)
and \( \exp\{-\beta \Delta \mu[r(u)]\} \) is called the influence functional which represents the solvent effects on the electron. In the continuum limit\(^{1}\),

\[
- \Delta \mu[r(u)] = \rho_s \hat{c}_{es}(0) + \frac{1}{2}(\beta \hbar)^{-2} \int_0^{\beta \hbar} du \int_0^{\beta \hbar} du' v(|r(u) - r(u')|),
\]

where \( \hat{c}_{es}(0) \) is the \( k = 0 \) spatial Fourier transform of \( c_{es}(r) \).

\[
v(|r(u) - r(u')|) = -\int dr' \int dr'' c_{es}(r', u) \chi_{ss}(|r' - r''|) c_{es}(|r'' - r|, u')
\]

Here \( r \) and \( u \) appear as independent coordinates, \( r \) is the distance between two sites and \( u \) measures the length along the contour of the polymer, and

\[
\chi_{ss}(|r - r'|) = \langle \delta \rho_s(r) \delta \rho_s(r') \rangle
\]

is the density-density correlation function of the unperturbed bath. In Eqs. (9) and (10), \( c_{es} \) is the direct correlation function. Its value is determined from the equation\(^{2}\)

\[
\rho_s h(r) = \int dr' \int dr'' \omega(|r - r'|) c_{es}(|r' - r''|) \chi_{ss}(r'')
\]

where

\[
\omega(|r - r'|) = (\beta \hbar)^{-1} \int d(u - u') \omega(|r - r'|; u - u').
\]

is the intrapolymer correlation function.

Eq. (12) is solved for \( c_{es} \) and \( h \) using suitable closure relation\(^{2}\). Since all sites of a ring polymer on the average are equivalent, the site dependence disappears from Eq.(12) and only the zero-frequency component \( \omega(|r|) \) of the equilibrium response function is required in Eq.(12).

To complete the evaluation of excess chemical potential, the electronic path integral still has to be performed. Following Feynman\(^{3}\) and Chandler et. al.\(^{4}\) the excess chemical potential for the fixed electronic path is mimicked by a Gaussian functional,

\[
- \beta \Delta \mu_{\text{ref}}[r(u)] = -\Gamma_0 + \frac{1}{2}(\beta \hbar)^{-2} \int_0^{\beta \hbar} du \int_0^{\beta \hbar} du' \Gamma(u - u') \times |r(u) - r(u')|^2
\]

where \( \Gamma(u - u') \) is a solvent-induced force constant between different sites on the electron polymer and \( \Gamma_0 \) merely determines the zero of energy. The Bogoliubov inequality provides a upper bound for the excess chemical potential,

\[
\Delta \mu \leq -\beta^{-1} \ln Z_{\text{ref}} + \langle \Delta \mu[r(u)] - \Delta \mu_{\text{ref}}[r(u)] \rangle_{\text{ref}}
\]
Here, $Z_{\text{ref}}$ is the electronic partition function for the Gaussian reference system and $< - >_{\text{ref}}$ means the average over the reference system weight determined by $S_o + \Delta \mu [r(u)]$. Minimizing the right hand side of Eq.(14) provides the optimal Gaussian reference system. This procedure leads to the following equations. The correlation function for the intrapolymer correlation in k-space:

$$\tilde{\omega}(k, \tau) = \exp\left[-\frac{k^2 R^2}{2D}\right] \tag{16}$$

where

$$R^2(\tau) = \langle |r(u) - r(u')|^2 \rangle = 4D \sum_{n \geq 1} A_n [1 - \cos(\Omega_n \tau)] \tag{17}$$

is the mean square displacement between two points on the electron path separated by a imaginary time incrementation $0 \leq u - u' \leq \beta \hbar$ with

$$A_n = (\beta m \Omega_n^2 + \gamma_n)^{-1} \tag{18}$$

where $\Omega_n = \frac{2\pi n}{\beta \hbar}$, and

$$\gamma_n = -(D \beta \hbar)^{-1} \int_0^{\beta \hbar} du [1 - \cos(\Omega_n u)] \int \frac{d^D k k^2}{(2\pi)^D} v(k) \exp(-k^2 R^2(u)/2D). \tag{19}$$

We solve Eq.(12) for $h$ and $c_{es}$ using closure relation

$$g = 0 \quad \text{for} \quad r \leq d \tag{20}$$

$$c_{es} = -\beta \epsilon \exp(-\alpha r) \frac{\alpha r}{\alpha r} \quad \text{for} \quad r > d \tag{21}$$

We can express Eq.(12) and the closure (20) in the variational form

$$\frac{\delta I_{RISM}}{\delta c_{es}} = 0 \tag{22}$$

where

$$I_{RISM} = \rho_s \hat{c}_{es}(0) + \frac{1}{2} \int \frac{d^D k}{(2\pi)^D} \hat{c}_{es}^2(k) \hat{\chi}_{ss}(k) \tilde{\omega}(k) \tag{23}$$

where $\hat{c}_{es}(0)$ is the $k = 0$ spatial Fourier transform of $c_{es}(r)$, $D$ is the dimensionality of the space, $d^D k$ is the dimensionality dependence volume element, $u$ labels the beads in the polymer ring ($0 \leq u \leq \beta \hbar$), $m$ is the bare electron mass, and $v(k) = -\hat{c}_{es}^2(k) \hat{\chi}_{ss}(k)$
is the Fourier transform of the potential between beads, which is found in Eq.(10). The information about the electron-solvent atom interaction is contained in the closure relation.

In Eq.(11), \( \omega(r) \) is the intra polymer distribution function averaged over all beads of the ring polymer. In writing Eq.(11) it has been assumed that for each polymer configuration, the solvent sees only average polymer rather than individual beads. The intra polymer distribution function \( \omega(r, \tau) \) is determined in the polaron approximation. \( \omega(k, u) \) is the Fourier transform of \( \omega(r, u) \) and is given by

\[
\hat{\omega}(k, u) = \exp\left[-k^2 R^2(u)/2D\right]. \tag{24}
\]

Eq.(22) is solved self-consistently for a given solvent and model potential representing the electron-fluid particle interaction. This solution gives information about \( v(r) \), \( \omega(r) \), \( R(u) \), \( \gamma_n \) and \( g(r) \) \( [ = 1+h(r)] \). Note that the quantity \( R(u) \) is the root mean square (RMS) value of the displacement between two points on the electron path separated by a time increment \( 0 \leq u \leq \beta \hbar \). The characteristic size or breadth of the polymer is measured by \( R(\beta \hbar/2) \). This is a measure of the spread of the wave packet associated with the particle. Since in the CSR theory a periodic boundary condition, \( r(0) = r(\beta \hbar) \), has been imposed on the path of the electron, \( R(u) \) is found to be symmetric about \( u = \frac{1}{2} \beta \hbar \), i.e. it starts from zero at \( u = 0 \), attain a maximum value at \( u = \frac{1}{2} \beta \hbar \) and decreases for \( u > \frac{\beta \hbar}{2} \) reaching zero at \( u = \beta \hbar \). \( g(r) \) gives information about the average packing of solvent particles around the electron. The variational parameter \( \gamma_n \) measures the strength of the electron fluid coupling. Quantities such as average kinetic energy, potential energy and effective mass etc., can be expressed in terms of \( \gamma_n \) as

\[
\langle K.E. \rangle = \frac{D}{2} k_B T \left[ 1 + \frac{\gamma_n}{\beta m \Omega_n^2 + \gamma_n} \right]. \tag{25}
\]

\[
\langle P.E. \rangle = \rho_s \int d\mathbf{r} u_{es}(|\mathbf{r}|)g(|\mathbf{r}|). \tag{26}
\]

\[
\frac{m}{m^*} = 24 \sum_{n \geq 0} \frac{1}{(4\pi^2 n^2 + \gamma_n \lambda^2_e)^{-1}}. \tag{27}
\]

In this equation \( m^* \) is the effective mass of the solvated electron. As mentioned earlier, we need two input for this theory. One is electron-solvent and another is the density-density correlation function of solvent which is related to the structure factor of the solvent.
For $D$-dimensional hard sphere solvent under consideration the Percus-Yevic (PY) equation can be solved analytically for $D = 1\text{ and for } D = 3$. For $D = 2$ excellent results of thermodynamic and structural properties have been obtained by Baus and Colot. In the above $\hat{\omega}$, $\hat{c}_{es}$, and $\hat{\chi}$, are the spatial Fourier transform of $\omega$, $c_{es}$, and $\chi$.

### III. RESULTS AND DISCUSSIONS

In presenting our results we mainly focus on the imaginary time correlation function

$$R^2(\frac{1}{2}\beta \hbar) = \langle |r(\frac{1}{2}\beta \hbar) - r(0)|^2 \rangle = 4D \sum_{n \geq 1} A_n (1 - \cos \pi n)$$

and the electron-solvent radial distribution function. Note that $R(\frac{1}{2}\beta \hbar)$ gives a measure of the physical size of the electron chain or the spread of the wave packet associated with the electron. For a free particle,

$$R(\frac{1}{2}\beta \hbar) = \sqrt{D/4} \lambda_e.$$  

In Fig.1 we plot the reduced correlation length, $S \equiv R(\frac{1}{2}\beta \hbar)/\sqrt{D/4} \lambda_e$ which is the dispersion of the wavepacket associated with the solvated electron relative to the free particle in one, two and three dimension as a function of density for $\lambda_e = 15\sigma$, $\alpha = \sigma^{-1}$ and $d/\sigma = 0.29$ for several values of the attractive interaction, $\beta \epsilon$. From these figures we find that when the electron-solvent interaction is solely repulsive ($\beta \epsilon = 0.0$), the electron is always gets trapped inside a solvent cage as solvent density is increased in one and two dimensions. In three dimension [see Fig. (1C)] the repulsive interaction is not strong enough (because $d/\sigma = 0.29$) to localize the electron due to ordered structure formed when the solvent density is high. When the attractive interaction between electron and solvent atom is large ($\beta \epsilon \simeq 100$), the reduced correlation length of the electron is very small at very low solvent density and it stays almost constant upto $\rho^* \sim 0.5$. This behavior strongly indicates the electron is localized to a single atom irrespective of space dimensionality. As the space dimensionality increases, the range of the constant value of the solvent density decreases for example for $D=1$, $S$ is constant upto $\rho^* \simeq 0.6$. One interesting feature we have noted from Figs. 1A, 1B, and 1C is that as the attractive interaction increases, the reduced correlation length of the electron decreases as we increase the solvent density in the low-density regime, but the correlation turns upward to have a maximum in the middle density regime, and
finally the electron is trapped in the high density regime. If we carefully look at Figs.1, we
observe that as we increase the space dimensionality, we find these effect are pronounced for
large attractive interaction. The similar type of behavior has been observed for the other
values of $d/\sigma$. When $d/\sigma$ is less than 0.29 we found the reduced correlation length of the
electron decreases as we increase the attractive interaction $\beta\epsilon$ and is self trapped at
lower density. Opposite trend is found for increasing $d/\sigma$.

From Figs. 1[A], 1[B] and 1[C] it is clear that at the beginning when we start increasing the
attractive interaction ($\beta\epsilon \simeq 20$) the wave packet associated with the electron increases then
further increase of electron solvent attractive interaction i.e. when $\beta\epsilon > 50.0$ the electron is
localized on a single solvent atom. The reason behind the delocalized state at small values of
attractive interaction ($\beta\epsilon$) is the cancellation between the repulsive and attractive electron-
solvent interaction. In Fig. 2[A] to Fig.2[F] we plot the electron-solvent radial distribution
function for one, two and three dimension at various solvent density and attractive interaction
($\beta\epsilon$). Figs. 2 can be explained in consistent manner with the same physical picture given
for Figs. [1]. When the attractive interaction is weak, the electron pushes the solvent atoms
makes space to self-trap. When the attractive interaction is very large ($\beta\epsilon \geq 100.0$) the
electron is trapped on a single atom irrespective of space dimensionality, as evidenced by a
large peak in $g(r)$ [see Figs. 2[F]].

In Fig. 3[A], 3[B], and 3[C] we plot the reduced correlation length as a function of $\lambda_e/\sigma$
at $\beta\epsilon = 0$ for $D=1$, 2, and 3 respectively. In one and two dimension (Fig.3[A] and Fig.3[B])
we observed as we increase $\lambda_e$ the electron is trapped in the solvent cage. If we compare
Fig. 3A with Fig. 3B as the space dimensionality increases, the electron is strongly trapped
in the solvent cage. One interesting feature we found in Fig. 3[C] at $\rho^* \sim 0.7$ there is sharp
transition from delocalized to self-trapped state. In less than two dimension when there
is no attractive interaction, the electron will always be in a localized state but in three
dimension there is always a tendency the electron will be in delocalized state. On the
other hand, as the temperature is decreased, the electron has tendency to be in the localized
state. This competition between various length scales probably make the sharp transition
around $\lambda_e \sim 16\sigma$.

In Fig. [4A], [4B] and [4C] we plot the reduced correlation length as a function of density
($\rho^*$) for various values of $d/\sigma$. We found for low $d/\sigma$ (for example $d/\sigma = 0.15$) the attractive
interaction dominates and the electron is self-trapped in the low density regime. On the
other hand, when \( d/\sigma \) is large the self-trapping of the electron is dominated by repulsive interaction or self-trapping is by cage effect. In the case of electron in helium and xenon, the self-trapping of electron in helium and delocalized state of the electron in xenon has been explained on the basis of \( d/\sigma \) value when electron-solvent interaction is repulsive i.e. \( \beta \epsilon = 0 \).

IV. CONCLUDING REMARKS

The CSR theory for the excess electrons in simple fluid (consisting of spherical atoms) has been studied in one, two, and three dimension. The detailed study led us to the following conclusions:

1. The reduced correlation length, \( S \), is very sensitive to the nature of the electron-fluid atom interaction, thermal wavelength of the excess electron (\( \lambda_e \)) and a length associated with the mean volume occupied by each fluid atom which is related to \( \rho^* = \rho \sigma^{D} \), where \( \rho^* \) is the number density of the fluid atoms and \( \sigma \) is the effective diameter of a fluid atom. The behavior is interpreted in terms of an interplay among the length scales noted above. When the electron-solvent attractive interaction is very large, the density dependence of the size of the electron polymer relative to the free particle is dominated essentially by the pair attractive interaction, and the electron is trapped in a single solvent atom irrespective of the dimensionality (\( D \)). On the contrary, if the attractive interaction is absent, the electron is trapped in a cage formed by the solvent atoms at higher density. When the attractive interaction is low (\( \beta \epsilon \sim 10.0 \)) due to cancellation between repulsive and attractive interaction, the electron is delocalized irrespective of the dimensionality.

2. In the one dimensional case the reduced correlation length is almost independent of \( d/\sigma \) when electron-solvent attractive interaction is absent. On the other hand, in two and three dimensions, \( S \), the reduced correlation length of the electron is sensitive on the value of the \( d/\sigma \).

3. In three dimension we found when \( d/\sigma = 0.29 \) and \( \beta \epsilon = 0.0 \), the temperature dependence of the reduced correlation length, \( S \), shows a sharp transition (metal-insulator type) around \( \lambda_e/\sigma \sim 15 \) at \( \rho^* \sim 0.7 \).
4. The long range electron-solvent attraction dominates at low density, while hard core repulsion dominates at high densities. When both interactions are present, they can counterbalance each other. Consequently, at some intermediate density, the effective electron-solvent interaction can be quite small, resulting in the electron delocalization.

In the present work we have explored the electron self-trapping in simple liquid for various space dimension ($D=1,2,\text{ and }3$) which have same model potential (solvent-solvent interaction potential and electron-solvent interaction potential) in every space dimension. In every space dimension (i.e. $D=1,2,\text{ and }3$) we have in the model system considered here there is repulsive as well as attractive electron solvent interaction potential which is not considered in Refs. 25, 27, and 28. We have presented the dimensionality dependent result for self trapping behavior of electron in simple liquid.

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**APPENDIX A: $D$-SPACE DIMENSIONAL INTEGRATION**

In $D$-space we have for any function $f(x)$ depending only on the distance $x = |x|$, 

$$
\int dxf(x) = S_D \int_0^\infty dx x^{D-1} f(x), \quad (A.1)
$$

or on $x$ and one integration angle $\theta$, 

$$
\int dxf(x,\theta) = S_{D-1} \int_0^\infty dx x^{D-1} \int d\theta \sin^{D-2}\theta f(x,\theta), \quad (A.2)
$$

where $S_D = D V_D$ is the surface area of the unit sphere of volume $V_D = \pi^{D/2}/\Gamma(1 + D/2)$, where $\Gamma(1 + z) = z!$ is the $\Gamma$ function.

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FIG. 1: Density ($\rho^*$) dependence of reduced correlation length ($S$) for various values of attractive interaction ($\beta \epsilon$) with $\lambda e = 15\sigma$, $\alpha = \sigma^{-1}$ and $d/\sigma = 0.29$ (A) for one dimension ($D = 1$), (B) for two dimension ($D = 2$), and (C) for three dimension ($D = 3$).
FIG. 2: Electron-solvent radial distribution function $g(r_\ast)$ for an electron in $D$-dimensional fluid at various density ($\rho_\ast$) with $d/\sigma = 0.29$, $\lambda_e/\sigma = 15\sigma$, and $\alpha = \sigma - 1$ for various values of attractive interaction ($\beta \varepsilon$) and various dimensionalities.
FIG. 3: Temperature dependence of the reduced correlation length, $S$, relative to the free particle value at $\alpha = \sigma^{-1}$ and $d/\sigma = 0.29$ for various values of density 

- (A) for one dimension ($D = 1$),
- (B) for two dimension ($D = 2$), and
- (C) for three dimension ($D = 3$).

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FIG. 4: Density dependence of the reduced correlation length at $\beta_\epsilon = 50$, $\lambda_e = 15\sigma$, and $\alpha = \sigma - 1$ for various values of $d/\sigma$. [A] for one dimension, [B] for two dimensions, [C] for three dimensions.