Exact and approximate results for the polaron in one dimension

F. M. Peeters and M. A. Smondyrev*
University of Antwerp (UIA), Department of Physics, Universiteitsplein 1, B-2610 Antwerpen, Belgium
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The Frölich polaron confined to move in one space dimension and interacting with a three-dimensional lattice is studied. We calculate exact and approximate results for the ground-state energy and the effective mass. The following exact results were obtained. In (a) the weak-coupling limit for the energy $E=-\alpha'-[(3/2\sqrt{2})-1]\alpha'^2$, the mass $m^*/m_b=\frac{1}{2}\alpha'+[(5/2\sqrt{2})-1]/4$, and the average number of virtual phonons $N=\frac{1}{2}\alpha'+[(3/\sqrt{2})-2]\alpha'^2$, and in (b) the strong-coupling limit $E=-0.333\,088\alpha'^2$, $m^*/m_b=2.1254\alpha'^4$, and $N=0.666\,176\alpha'^2$. Here, α' is the normalized electron-phonon coupling constant, which was chosen such that $E=-\alpha'$ within second-order perturbation theory.

I. INTRODUCTION

One-dimensional polaron problems are relevant in semiconductor physics, where with state-of-the-art nanolithography it has become possible to confine electrons in one direction[1] (i.e., quantum wires), and in linear conjugated organic polymer conductors[2,3], e.g., *cis*- and *trans*-polyacetylene. The latter are much more strongly bound and are described by the small-polaron Hamiltonian.

In the present paper we will focus on the large polaron and we consider the extreme case of complete confinement into one dimension. The Hamiltonian is of the standard Fröhlich type, which was derived in Ref. 4 for the case of arbitrary spatial dimensions,

$$H=\frac{\mathbf{p}^2}{2m_b}+\sum_{\mathbf{k}}\hbar\omega_{\mathrm{LO}}a_{\mathbf{k}}^{\dagger}a_{\mathbf{k}}+\sum_{\mathbf{k}}(V_{\mathbf{k}}a_{\mathbf{k}}e^{i\mathbf{k}\cdot\mathbf{r}}+V_{\mathbf{k}}^{*}a_{\mathbf{k}}^{\dagger}e^{-i\mathbf{k}\cdot\mathbf{r}}) , \tag{1}$$

where

$$|V_k|^2=\Gamma\left[\frac{n}{2}\right]2^{n-1/2}\pi^{n/2-1}\frac{\alpha'}{Vk^{n-1}} , \tag{2}$$

with $\alpha'=\alpha\sqrt{\pi}\Gamma[(n-1)/2]/2\Gamma(n/2)$ and α is the standard[5] dimensionless three-dimensional (3D) electron-phonon coupling constant. Note that for $n\to 1$ we have $\alpha'=\alpha/(n-1)$. The fact that the polaron characteristics diverge for $n=1$ is a consequence of the Coulomb nature of this problem. By using α' instead of α as the electron-phonon coupling constant, we have regularized all the expressions and finite results are found for the energy and the mass.

Degani *et al.*[6] have calculated the ground-state energy and effective mass of such 1D polarons by using the Feynman path-integral formalism. They defined a dimensionless electron-phonon coupling constant α_{op} which is related to ours $\alpha'=2\pi\alpha_{\mathrm{op}}$. Our definition of the electron-phonon coupling constant is such that the ground-state energy in second-order perturbation theory is given by $E=-\alpha'$ in all space dimensions. Degani *et al.*[6] found that the properties of the optical polaron are a continuous function of the electron-phonon coupling constant. In fact this conclusion is a direct consequence of a scaling relation[7] which was recently proved for the Feynman approximation and which allows us to obtain the ground-state energy and the effective mass in n dimensions[8] from the known results in 3D:

$$E_{n\mathrm{D}}(\alpha')=\frac{n}{3}E_{3\mathrm{D}}\left[\frac{3}{n}\alpha'\right] , \tag{3a}$$

$$\left[\frac{m^*(\alpha')}{m_b}\right]_{n\mathrm{D}}=\left[\frac{m^*\left[\frac{3}{n}\alpha'\right]}{m_b}\right]_{3\mathrm{D}} . \tag{3b}$$

As a consequence all the conclusions[9] concerning the continuous behavior of E and m^* in 3D when the coupling constant goes from the weak- to the strong-coupling limit are also satisfied for $n=1$ and the conclusions of Ref. 6 are a natural consequence of the scaling relations [(3a) an (3b)].

The aim of the present paper is to present exact results for the 1D polaron ground-state energy and effective mass in the weak- (up to fourth-order perturbation theory which is presented in Sec. II) and strong-coupling limit (see Sec. III). These results will be compared with different approximate results as, e.g., the Feynman theory and the $1/n$ expansion[10] in Sec. IV.

II. WEAK-COUPLING LIMIT

The polaron ground-state energy and effective mass will be calculated up to the second-order in the electron-phonon coupling constant. In Ref. 11 a diagrammatic technique for the moving 3D large polaron has been developed. These results were generalized to the multidimensional case in Ref. 12. For the details we refer to Refs. 11 and 12. Here only the results will be presented. For convenience we use units such that $\hbar=m_b=\omega_{\mathrm{LO}}=1$.

The energy of a moving polaron is expanded within conventional perturbation theory

$$E(\mathbf{p}_0)=E_0(\mathbf{p}_0)+\sum_{n=1}^{\infty}\alpha'^n E_n(\mathbf{p}_0)\ , \tag{4}$$

where $E_0(\mathbf{p}_0)=\mathbf{p}_0^2$ is the kinetic energy of a free electron and $\mathbf{p}_0=\mathbf{p}/\sqrt{2}$ with $\mathbf{p}$ the total conserving momentum of the system. In the limit of a slow-moving polaron, we have

$$E(\mathbf{p}_0)=E+\mathbf{p}_0^2/m^*+\theta(p_0^4)\ , \tag{5}$$

with $E=\sum_{n=1}^{\infty}\alpha'^n E_n$ the polaron energy at zero momentum and $m^*=1+\sum_{n=1}^{\infty}\alpha'^n m_n$ its corresponding mass.

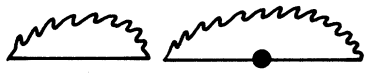
To the first order in the electron-phonon coupling constant the polaron energy is given by the diagram

$$=\alpha' E_1(p_0)=-\alpha'\frac{1}{\pi}\int_{-\infty}^{+\infty}dk\frac{1}{k^2-2p_0k+1}=-\frac{\alpha'}{(1-p_0^2)^{1/2}}\ . \tag{6}$$

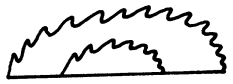
The second-order term is given by a sum of three diagrams, one of which is unconnected.[11] Introducing the notations for the electron propagators in states with 1 and 2 virtual phonons, respectively,

$$P(k)=\frac{1}{k^2-2p_0k+1}\ ,$$
$$P(q,k)=\frac{1}{(q+k)^2-2p_0(q+k)+2}\ , \tag{7}$$

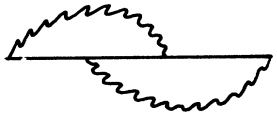
we obtain



$$=-\alpha'^2 E_1(p_0)\frac{1}{\pi}\int_{-\infty}^{+\infty}dk\,P^2(k)=\frac{\alpha'^2}{2(1-p_0^2)^2}\ ,$$



$$=-\left[\frac{\alpha'}{\pi}\right]^2\int_{-\infty}^{+\infty}dk\,dq\,P^2(q)P(q,k)=-\frac{\alpha'^2}{2(1-p_0^2)^{3/2}(2-p_0^2)^{1/2}}\ , \tag{8}$$



$$=-\left[\frac{\alpha'}{\pi}\right]^2\int_{-\infty}^{+\infty}dk\,dq\,P(q)P(k)P(q,k)=-\alpha'^2\left[\frac{(1-p_0^2)^{1/2}}{(2-p_0^2)^{1/2}}+\frac{1}{2(1-p_0^2)}-1\right]\ ,$$

With Eqs. (6)–(8) we readily find the coefficients of the weak-coupling expansions (5) for the polaron energy and effective mass

$$E_1=-1,\quad m_1=\tfrac{1}{2}\ ,$$
$$E_2=-(\tfrac{3}{4}\sqrt{2}-1),\quad m_2=(5\sqrt{2}-4)/16\ . \tag{9}$$

The average virtual number of phonons N can be obtained from the polaron energy

$$N(p_0)=\left[1-\frac{3}{2}\alpha\frac{\partial}{\partial\alpha}-\frac{1}{2}p_0\frac{\partial}{\partial p_0}\right]E(p_0)\ , \tag{10}$$

which is an exact relation which was proved in Ref. 11. Using the above results for the energy, we can write the general perturbation expansion

$$N(p_0)=\sum_{n=1}^{\infty}\alpha'^n N_n(p_0)\ , \tag{11}$$

where the first term is

$$N_1=\tfrac{1}{2}\ , \tag{12}$$

and to the second order in the coupling constant

$$N_2=(3\sqrt{2}-4)/2\ , \tag{13}$$

in case the electron is at rest ($p_0=0$).

III. STRONG-COUPLING LIMIT

For $\alpha\gg 1$ the electron motion is much faster than the lattice frequency ω_{LO} and as a consequence the adiabatic approximation becomes exact. Following Pekar[13] the ground-state wave function of the electron $|\psi\rangle$ is determined by the integrodifferential equation

$$\left[\frac{\mathbf{p}^2}{2m_b}+\sum_{\mathbf{k}}|V_{\mathbf{k}}|^2(|\langle\psi|e^{i\mathbf{k}\cdot\mathbf{r}}|\psi\rangle|^2-2e^{-i\mathbf{k}\cdot\mathbf{r}}\langle\psi|e^{i\mathbf{k}\cdot\mathbf{r}}|\psi\rangle)\right]\psi(\mathbf{r})=E\psi(\mathbf{r})\ , \tag{14}$$

which was obtained by using the product ansatz $|\Phi\rangle=|\psi\rangle|\phi\rangle$ for the electron-phonon ground-state wave function and optimizing with respect to the phonon wave function $|\phi\rangle$. Inserting Eq. (2) into Eq. (14) and using the transformation $\mathbf{r}\rightarrow\mathbf{r}/\sqrt{2}\alpha'$ and $\mathbf{k}\rightarrow\mathbf{k}\sqrt{2}\alpha'$ we obtain

$$\left[-\Delta-2\frac{\Gamma(n/2)}{\pi^{1+n/2}}\int\frac{d^nk}{k^{n-1}}e^{-i\mathbf{k}\cdot\mathbf{r}}\rho(\mathbf{r})\right]\psi(\mathbf{r}) =(-A+V_a)\psi(\mathbf{r}) , \quad (15a)$$

with

$$V_a=\frac{\Gamma(n/2)}{\pi^{1+n/2}}\int\frac{d^nk}{k^{n-1}}|\rho(\mathbf{k})|^2 , \quad A=-\frac{E}{\alpha'^2} , \quad (15b)$$

and $\rho(\mathbf{k})=\langle\psi|e^{i\mathbf{k}\cdot\mathbf{r}}|\psi\rangle=\int d\mathbf{r}|\psi(\mathbf{r})|^2e^{i\mathbf{k}\cdot\mathbf{r}}$. Note that the α' dependence has been scaled out of the problem and in the strong-coupling limit the ground-state energy is proportional to α'^2 irrespective of the dimension of the problem. It will be more convenient to convert the problem into a variational one

$$A=-\frac{E}{\alpha'^2}=\langle\psi|\Delta|\psi\rangle+\frac{\Gamma(n/2)}{\pi^{1+n/2}}\int\frac{d^nk}{k^{n-1}}|\langle\psi|e^{i\mathbf{k}\cdot\mathbf{r}}|\psi\rangle|^2 . \quad (16)$$

In the adiabatic limit Miyake[14,15] obtained an expression for the effective mass which we generalized in Ref. 16 to arbitrary space dimensions

$$\frac{m^*}{m_b}=2\sum_{\mathbf{k}}|V_{\mathbf{k}}|^2(\mathbf{k}\cdot\mathbf{e}_t)^2|\langle\psi|e^{i\mathbf{k}\cdot\mathbf{r}}|\psi\rangle|^2 , \quad (17)$$

with $\mathbf{e}_t$ a unit vector in an arbitrary direction. Inserting the expression for $|V_{\mathbf{k}}|^2$ into Eq. (17) and applying the transformations $\mathbf{r}\rightarrow\mathbf{r}/\sqrt{2}\alpha'$ and $\mathbf{k}\rightarrow\mathbf{k}\sqrt{2}\alpha'$ this becomes

$$\frac{m^*}{m_b}=4\frac{\Gamma(n/2)}{\pi^{1+n/2}}\alpha'^4\int_{-\infty}^{\infty}\frac{d^nk}{k^{n-1}}(\mathbf{k}\cdot\mathbf{e}_t)^2|\langle\psi|e^{i\mathbf{k}\cdot\mathbf{r}}|\psi\rangle|^2 . \quad (18)$$

The above equations (15) and (16) are a generalization of Eqs. (8)–(10) of Ref. 7 to arbitrary space dimensions. In the present paper we are interested in the 1D polaron and in this case Eq. (16) takes the form

$$A=\langle\psi|\Delta|\psi\rangle+\frac{1}{\pi}\int_{-\infty}^{\infty}dk|\langle\psi|e^{ikx}|\psi\rangle|^2 , \quad (19)$$

and the mass becomes

$$M=\frac{m^*}{m_b}\frac{1}{\alpha'^4}=\frac{4}{\pi}\int_{-\infty}^{\infty}dk\,k^2|\langle\psi|e^{ikx}|\psi\rangle|^2 . \quad (20)$$

It is possible to solve the integrodifferential equation Eq. (15a) numerically and to find the wave function and energy $A=-E/\alpha'^2$. We have chosen an alternative route and propose different functional forms for the electron wave function and minimize the energy (16) to obtain the optimal approximation. We have taken the following.

(1) An exponential trial wave function: $\psi=\sqrt{b}\,e^{-b|x|}$ which gives $b=0.5$ $A=0.25$, and $M=2$.

(2) A Gaussian: $\psi=(2b/\pi)^{1/4}e^{-bx^2}$ which after the variational calculation gives $b=1/\pi$ and $A=1/\pi=0.318\,309\,9$, and $M=16/\pi^2=1.6211$.

(3) The Pekar[13] wave function: $\psi=(2b/5)^{1/2}(1+b|x|)e^{-b|x|}$ which results in $b=\frac{103}{80}=1.2875$, $A=\frac{10\,609}{3200}=0.331\,531\,2$, and $M=2.2196$.

(4) The Pekar-type ansatz: $\psi=N[1+b|x|+a(bx)^2]e^{-b|x|}$ with N a normalization constant and $\alpha=0.2624$ and $b=1.6392$ and $A=0.332\,547\,8$, and $M=2.1064$.

In order to find the exact result for $A=-E/\alpha'^2$ we start from the knowledge that the electron wave function has to decay exponentially at large distances. This can be found from Eq. (15a) and is a direct consequence of the Coulombic nature of the electron-phonon interaction. Thus the electron wave function has to be of the form $\psi(x)=\sum_{l=0}^{\infty}a_l|x|^le^{-b|x|}$. We will cut off the series when the energy is determined to a sufficient accuracy. We found that

$$\psi(x)=N[1+b|x|+a(bx)^2+c(b|x|)^3+d(bx)^4]e^{-b|x|} \quad (21)$$

is able to determine the energy with sufficient accuracy. A numerical minimalization of the ground-state energy leads to $a=0.3516$, $b=1.859$, $c=-0.002\,982$, and $d=0.008\,369$ and for the energy $E/\alpha'^2=-0.333\,087\,7$ and the mass $M=2.1254$. For the average number of phonons we get from Eq. (10) $N/\alpha'^2=-2(E/\alpha'^2)=0.666\,175$. The resulting wave function is shown in Fig. 1 together with the Gaussian and exponential wave

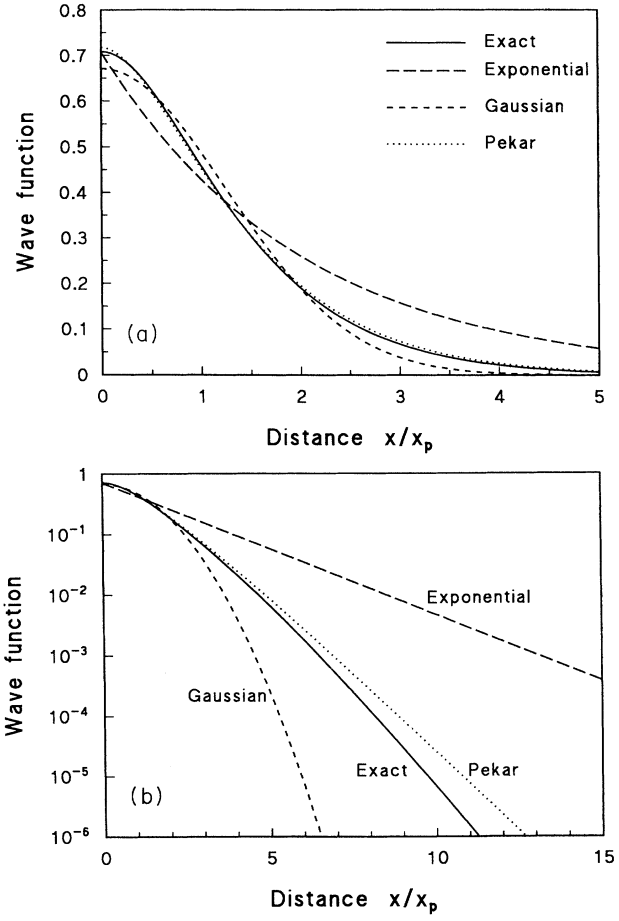


FIG. 1. Normalized wave function for the 1D polaron in the strong-coupling limit for different approximations and for the exact theory. The distance is in units of $x_p=\sqrt{\hbar/2m_b\omega_{LO}}(1/\alpha')$.

function. Around the origin [see Fig. 1(a)] the exact wave function is quadratic while at large distances [see Fig. 1(b)] the wave function decays exponentially.

IV. APPROXIMATE RESULTS AND CONCLUSION

The 1D optical polaron has been studied by Degani *et al.*[6] using the Feynman path-integral approach. In the weak-coupling limit they reported results up to the first order in the coupling constant ($\alpha_{\rm op}=\alpha'/2\pi$): $E=-2\pi\alpha_{\rm op}=-\alpha'$, and $m^*/m_b=1+2\pi\alpha_{\rm op}=1+\alpha'$. The coefficient m_1 differs from that of Eq. (9) by a factor of 2 which we believe is an error of Ref. 6. In the strong-coupling limit Degani *et al.*[6] obtained $E=-4\pi\alpha_{\rm op}=-\alpha'^2/\pi$ and $m^*/m_b=256\pi^2\alpha_{\rm op}^4=\alpha'^4\times16/\pi^2$, which is our Gaussian result given in the preceding section.

But the Feynman result can be obtained without any sophisticated calculations just through the scaling laws (3). Thus from the well-known Feynman results[17] for a 3D polaron in the weak-coupling limit $E_{\rm 3D}=-\alpha-\frac{1}{81}\alpha^2$, and $m^*_{\rm 3D}=1+\frac{1}{6}\alpha+\frac{2}{81}\alpha^2$, and the strong-coupling limit $E_{\rm 3D}=-\alpha^2/3\pi-(3ln2+\frac{3}{4})$, and for the mass $m^*_{\rm 3D}=(16/81\pi^2)\alpha^4-\alpha^2(4/3\pi)(2ln2+1)$, one readily obtains the results for the 1D polaron in the weak-coupling limit

$$E=-\alpha'-\tfrac{1}{27}\alpha'^2,\quad m^*=1+\tfrac{1}{2}\alpha'+\tfrac{2}{9}\alpha'^2\ , \tag{22}$$

and the strong-coupling limit

$$E=\frac{1}{\pi}\alpha'^2-(\ln2+\tfrac{1}{4}),\quad m^*=\frac{16}{\pi^2}\alpha'^4-\alpha'^2\frac{12}{\pi}(2ln2+1)\ . \tag{23}$$

The scaling relations (3) were proved for the Feynman approximation[8] and, in general for Gaussian-type approximations.[10] It can be generalized easily to arbitrary dimensions

$$E_{n\rm D}(\alpha')=\frac{n}{l}E_{l\rm D}\left[\frac{l}{n}\alpha'\right],\qquad m^*_{n\rm D}(\alpha')=m^*_{l\rm D}\left[\frac{l}{n}\alpha'\right], \tag{24}$$

and used to obtain approximate results in 1D from exact ones in, e.g., 2D and 3D. For the 3D polaron we have the exact results

$$(E_2)_{\rm 3D}=-0.015\,919\,62\ ,\quad (m_2)_{\rm 3D}=0.023\,627\,63\ , \tag{25}$$
$$(A)_{\rm 3D}=0.108\,513,\quad (M)_{\rm 3D}=0.022\,701\,9\ ,$$

and for the 2D polaron

$$(E_2)_{\rm 2D}=-0.025\,927\,67,\quad (m_2)_{\rm 2D}=0.051\,566\,33\ , \tag{26}$$
$$(A)_{\rm 2D}=0.164\,026,\quad (M)_{\rm 2D}=0.120\,370\ .$$

Now we use the scaling laws (24) for $n=1$ and $l=2,3$, and insert Eqs. (25) and (26). The results are presented in Tables I and II. As intuitively expected the closer the starting dimension is to $n=1$ the better the approximation we obtain from the scaling argument.

In Ref. 10 a new approach to the polaron problem has been developed which is based on an expansion in inverse powers of the number n of space dimensions. In such an approach there are no limitations on α. The results for the coefficients E_2 and A in the weak- and strong-coupling limits are as follows:

$$E_2=-\left[\frac{1}{2n\sqrt{\pi}}\right]^2\left[n\left[\pi-\frac{8}{3}\right]+\left[\frac{108}{5}-\frac{27\pi}{4}\right]+\theta\left[\frac{1}{n}\right]\right],$$
$$A=\left[\frac{1}{2n\sqrt{\pi}}\right]^2\left[4n+(13-4\sqrt{10})+\theta\left[\frac{1}{n}\right]\right]. \tag{27}$$

It was proven that the leading term coincides in 3D with the approximation of Adamowski *et al.*[18] and Saitoh,[19] which is the best Gaussian-type upper estimate where an arbitrary quadratic trial action was introduced in a path-integral evaluation of the ground-state energy. In the strong-coupling limit the leading approximation A coincides with the Feynman result, which in the weak-coupling limit E_2 is slightly improved. For $n=1$ we obtain

$$E_2=\frac{23}{16}-\frac{71}{15\pi},\quad A=(17-4\sqrt{10})/4\pi\ . \tag{28}$$

These results are a lower bound on the energy. Thus absolute values of E_2 and A in Eq. (27) are larger and they are very close to the exact values as seen from Tables I and II.

The $1/n$ expansion for the effective mass gives

TABLE I. The second-order coefficient for the ground-state energy E_2 and the polaron mass m_2.

Theory	$-E_2$	m_2
Feynman	0.037 037	0.222 222
Scaling from 3D	0.047 759	0.212 649
Scaling from 2D	0.051 855	0.206 265
$1/n$ leading term	0.037 793	0.226 760
$1/n$ expansion	0.069 167	
Exact	0.060 660	0.191 942

TABLE II. The ground-state energy and polaron mass in the strong-coupling limit to leading order in α'.

Theory	$A=-E/\alpha'^2$	$M=(m^*/m_b)/\alpha'^4$
Exponential	0.25	2.0
Gaussian	0.318 310	1.6211
($1/n$ leading term)		
Pekar	0.331 531	2.2196
Modified Pekar	0.332 548	2.1064
Scaling from 3D	0.325 539	1.8389
Scaling from 2D	0.328 052	1.9259
$1/n$ expansion	0.346 233	
Exact	0.333 088	2.1254

$$m_2 = \left[\frac{1}{2n\sqrt{\pi}}\right]^2 \left[2(3\pi-8)+\theta\left[\frac{1}{n}\right]\right], \qquad M = \left[\frac{1}{2n\sqrt{\pi}}\right]^2 \left[256+\theta\left[\frac{1}{n}\right]\right]. \tag{29}$$

At $n=1$ we get for M the Feynman-type result, and for m_2 a slightly different value. The next correction in the $1/n$ expansion was not obtained.

In conclusion, we presented calculations for the exact results of a 1D polaron energy, mass, and number of virtual phonons in the limits of weak and strong electron-phonon coupling. These results are compared with results from different approximate theories.

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*Present address: Joint Institute for Nuclear Research (Dubna), Head Post Office Box 79, Moscow, U.S.S.R.

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