Gauss, Wannier, and ultralocalized functions

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We study the localization properties of Wannier functions composed of Gaussian orbitals and of corresponding ultralocalized functions. In particular, we prove that finding specific ultralocalized functions is equivalent to solving Lamé's equation. [S0163-1829(98)00736-X]

I. INTRODUCTION

In a recent publication we have investigated Bloch[1] and Wannier[2] functions composed of Gaussian orbitals.[3] Since these Bloch functions can be expressed in terms of θ functions,[3,4] a detailed analysis of their properties is possible.

Let us agree on the following terminology. We call a function $\psi(k,x)$ a Bloch function if it has the transformation property $\psi(k,x-n)=e^{ikn}\psi(k,x)$ (we assume that the lattice constant $a=1$). It would be more precise to call such a function a quasi-Bloch function since usually a Bloch function is meant to be an eigenfunction of a certain periodic Hamiltonian. However, to keep the terminology shorter we just say Bloch function instead of quasi-Bloch function. Since we deal only with such quasi-Bloch functions this should not lead to any confusion. Correspondingly, we call a function $W(x)$ a Wannier function if it fulfills the usual orthogonality relation $\int_{-\infty}^{\infty}W(x-n)^*W(x-m)dx=\delta_{nm}$, but again it is not meant to be related to a certain Hamiltonian.

Usually the Wannier functions are not the best localized functions for a given band. So one often is interested in finding better localized functions, which of course lack the orthogonality properties. As a measure of localization one can use the falloff at infinity. From this point of view the original Gauss functions are already the best localized ones. However, one can also use the uncertainty Δx as a measure of localization. It turns out that suitably chosen Wannier functions have the same Δx as the original Gaussians. We construct several ultralocalized functions, i.e., functions whose Δx is smaller than that of the corresponding Gauss functions. We prove that finding ultralocalized functions with the minimal Δx is equivalent to solving Lamé's equation. Since it is not possible to solve this equation exactly, we consider some approximations.

The paper is organized as follows. We start with a short review of the most important properties of the Bloch and Wannier functions composed of Gaussian orbitals (Sec. II). In Sec. III we discuss the localization properties of the Wannier functions. The following sections deal with the ultralocalized functions. In Sec. IV A we investigate the ultralocalized functions with the minimal Δx. In particular we show that the problem of finding these ultralocalized functions can be reduced to solving Lamé's equation. The following sections deal with several approximate solutions of Lamé's equation and the corresponding ultralocalized functions. One of these ultralocalized functions is very remarkable: If we start with a rather extended Gaussian $e^{-\beta x^2}$, where β is small, then we can construct an ultralocalized function that is the sum of a more localized Gaussian and a small rest: $e^{-(\beta/\alpha)x^2}+\varepsilon(x)$ with $\alpha<1$.

II. BLOCH AND WANNIER FUNCTIONS

We start with the one-dimensional Gaussian orbitals

$$G^{\beta}(x)=\left(\frac{2\beta}{\pi}\right)^{1/4}e^{-\beta x^2} \tag{1}$$

and use them to construct Bloch functions.[3,4] These Bloch functions may be expressed in terms of θ functions[5–7]

$$\begin{aligned}\phi_k^{\beta}(x)&=\frac{1}{\sqrt{2\pi}}\frac{1}{\sqrt{\theta_3\left(\frac{k}{2}\middle|\frac{i\beta}{2\pi}\right)}}\left(\frac{2\beta}{\pi}\right)^{1/4}\\&\quad\times e^{-\beta x^2}\theta_3\left(\frac{k}{2}-i\beta x\middle|\frac{i\beta}{\pi}\right)\\&=e^{ikx}\frac{1}{\sqrt{2\pi}}\frac{\theta_3\left(\frac{i\pi}{\beta}\frac{k}{2}+\pi x\middle|\frac{i\pi}{\beta}\right)}{\sqrt{\theta_3\left(\frac{i\pi}{\beta}k\middle|\frac{2i\pi}{\beta}\right)}}.\end{aligned} \tag{2}$$

The Bloch functions are normalized in such a way that $\int_0^1dx|\phi_k^{\beta}(x)|^2=1/2\pi$ holds. We adopt the following conventions for the Wannier functions $W_n^{\beta}:\mathbb{R}\rightarrow\mathbb{R}$:

$$W_n^{\beta}(x)=\frac{1}{(2\pi)^{1/2}}\int_{-\pi}^{\pi}dk\ \phi_k^{\beta}(x)e^{-ikn}, \tag{3}$$

which can be written as

$$W_0^\beta(x)=\frac{1}{2\pi}\int_{-\infty}^{\infty}e^{ikx}\frac{1}{\theta_3\left(\frac{i\pi k}{\beta}\middle|\frac{2\pi i}{\beta}\right)^{1/2}}dk$$

$$=\frac{1}{2\pi}\left(\frac{2\pi}{\beta}\right)^{1/4}\int_{-\infty}^{\infty}e^{ikx}\frac{e^{-(1/4\beta)k^2}}{\theta_3\left(\frac{k}{2}\middle|\frac{i\beta}{2\pi}\right)^{1/2}}dk. \quad (4)$$

It can be shown[8,3] that the Bloch functions ϕ_k^β are analytic functions of k in the strip $\{k:|\mathrm{Im}\,k|<\beta/2\}$ and thus the Wannier functions fall off exponentially:[9] $|W_0^\beta(x)|\leqslant e^{-(\beta/2)|x|}B^\beta$, where B^β is an appropriate constant.

III. LOCALIZATION PROPERTIES OF THE WANNIER FUNCTIONS

Although the original Gauss functions fall off much faster than the Wannier functions, the uncertainty Δx is the same for both Gauss and Wannier functions, namely,

$$\Delta x_{W_n^\beta}=\sqrt{\langle W_n^\beta,x^2W_n^\beta\rangle-\langle W_n^\beta,xW_n^\beta\rangle^2}=\Delta x_{G^\beta}=\frac{1}{\sqrt{4\beta}}. \quad (5)$$

This is due to the better localization of the Wannier functions near the origin. This can be shown as follows: Due to periodicity with respect to k we have

$$W_0^\beta(0)=\frac{1}{(2\pi)^{1/2}}\int_{-\pi}^{\pi}dk\,\frac{1}{2}[\phi_k^\beta(0)+\phi_{k-\pi}^\beta(0)]$$

$$>\sqrt{\theta_3\left(0\middle|\frac{2i\beta}{\pi}\right)}G^\beta(0)>G^\beta(0), \quad (6)$$

since the following inequality for the integrand is valid:

$$\frac{1}{2}[\phi_k^\beta(0)+\phi_{k+\pi}^\beta(0)]\geqslant\frac{1}{\sqrt{2\pi}}G^\beta(0)\sqrt{\theta_3\left(0\middle|\frac{2i\beta}{\pi}\right)}, \quad (7)$$

which can be proved easily by using the formula

$$\left[\theta_3\left(\frac{k}{2}\middle|\frac{i\beta}{\pi}\right)\right]^2=\frac{1}{2}\left[\theta_3\left(\frac{k}{2}\middle|\frac{i\beta}{2\pi}\right)\theta_3\left(0\middle|\frac{i\beta}{2\pi}\right)+\theta_4\left(\frac{k}{2}\middle|\frac{i\beta}{2\pi}\right)\theta_4\left(0\middle|\frac{i\beta}{2\pi}\right)\right] \quad (8)$$

and the inequality

$$(CAB+DA^2)^{1/2}+(CAB+DB^2)^{1/2}\geqslant2(C+D)^{1/2}(AB)^{1/2}, \quad (9)$$

which is valid if A, B, C, and D are non-negative real numbers and where the inequality sign is valid if $D>0$ and $A\neq B$. In a similar way one can prove

$$W_0^\beta(0)>\sqrt{\theta_3\left(0\middle|\frac{2i\pi}{\beta}\right)}>1. \quad (10)$$

Note in passing that our particularly chosen Wannier functions have minimal uncertainty Δx in the following sense: For any other Wannier function composed of Gaussian orbitals the uncertainty Δx is larger.[3]

IV. ULTRALOCALIZED FUNCTIONS

In the preceding section we have discussed the uncertainty Δx for Gauss and Wannier functions and we have seen that in both cases $\Delta x=1/\sqrt{4\beta}$ is valid. The fact that the Wannier functions are better localized at the origin whereas the Gauss functions fall off faster for $x\to\pm\infty$ suggests that we can find a linear combination of Gauss functions whose uncertainty Δx is smaller, i.e., $\Delta x<1/\sqrt{4\beta}$. This can be achieved by constructing a function with the following two properties: It is better localized than the Gauss function at the origin and its exponentially damped oscillating tail is smaller than that of the Wannier functions. Let us call a function ultralocalized if $\Delta x<1/\sqrt{4\beta}$ holds. Note that these ultralocalized functions do not have the nice orthogonality properties of the Wannier functions, but in practical applications one often does not lay stress on these orthogonality properties.[10]

In the following sections we need not only the expectation value $\langle x^2\rangle$ for ultralocalized functions but also the matrix elements $\langle W_n^\beta,x^2W_m^\beta\rangle$ for the definition of Anderson's ultralocalized functions. Thus we compute $\langle\psi,x^2\chi\rangle$ in general, where ψ and χ are linear combinations of the Wannier functions W_n^β, namely,

$$\psi(x)=\frac{1}{\sqrt{2\pi}}\int_{-\pi}^{\pi}dk\,f(k)\phi_k^\beta, \quad (11)$$

$$\chi(x)=\frac{1}{\sqrt{2\pi}}\int_{-\pi}^{\pi}dk\,g(k)\phi_k^\beta. \quad (12)$$

We assume that both ψ and χ are in the domain of definition of x^2; in particular f and g are periodic and their derivatives exist and are absolutely continuous. Thus we have

$$\langle\psi,x^2\chi\rangle=\frac{1}{4\beta}\frac{1}{2\pi}\int_{-\pi}^{\pi}dk\,f^*(k)g(k)+\frac{1}{2\pi}\int_{-\pi}^{\pi}dk\,\frac{\partial f^*(k)}{\partial k}\frac{\partial g(k)}{\partial k}+\frac{1}{8\pi}\int_{-\pi}^{\pi}dk\,f^*(k)g(k)\,\frac{\partial^2}{\partial k^2}\ln\,\theta_3\left(\frac{k}{2}\middle|\frac{i\beta}{2\pi}\right). \quad (13)$$

A. Ultralocalized functions with minimal Δx

Before we construct some ultralocalized functions we want to derive an equation for the ultralocalized function that has the minimal uncertainty Δx. We restrict our discussion to symmetric functions, thus the uncertainty Δx is simply given by $\Delta x=\sqrt{\langle x^2\rangle}$. In fact, this is no restriction, as we discuss below. Let these ultralocalized functions be given by

$$u^\beta(x)=\sum_n c_n^\beta W_n^\beta=\frac{1}{\sqrt{2\pi}}\int_{-\pi}^{\pi}dk\,f^\beta(k)\phi_k^\beta, \quad (14)$$

where we assume that u^β is properly normalized, i.e., that each of the following equations holds:

$$\|u^\beta\|=1\Leftrightarrow\sum_{n=-\infty}^{\infty}|c_n^\beta|^2=1\Leftrightarrow\frac{1}{2\pi}\int_{-\pi}^{\pi}|f^\beta(k)|^2=1. \quad (15)$$

Then $\langle x^2\rangle$ with respect to u^β reads

$$\langle x^2\rangle=\frac{1}{4\beta}+\frac{1}{2\pi}\int_{-\pi}^{\pi}dk\left|\frac{\partial f^\beta(k)}{\partial k}\right|^2+\frac{1}{8\pi}\int_{-\pi}^{\pi}dk\,|f^\beta(k)|^2\,\frac{\partial^2}{\partial k^2}\ln\,\theta_3\left(\frac{k}{2}\middle|\frac{i\beta}{2\pi}\right). \quad (16)$$

Hence the minimum of $\langle x^2\rangle$ is obtained for the function f^β that fulfills the Euler-Lagrange equation

$$-\frac{\partial^2 f^\beta(k)}{\partial k^2}+\left[\frac{1}{4\beta}+\frac{1}{4}\frac{\partial^2}{\partial k^2}\ln\,\theta_3\left(\frac{k}{2}\middle|\frac{i\beta}{2\pi}\right)\right]f^\beta(k)=\lambda^\beta f^\beta(k) \quad (17)$$

and is periodic. Note that this implies that f^β is even. This equation is Lamé's equation, which is well known in mathematical literature. The usual form[7]

$$\frac{d^2y}{du^2}(u)-n(n+1)\mathcal{P}(u)y(u)=\mu y(u) \quad (18)$$

is obtained if we set $u=k/2+\pi/2+i\beta/4$, $y(u)=f^\beta(k)$, and $n=-\frac{1}{2}$ and choose μ appropriately. Here $\mathcal{P}(u)$ is Weierstrass's elliptic function,[5,7] which is defined by

$$\mathcal{P}(u)=\mathcal{P}(u;\omega_1,\omega_3):=\left(\frac{\pi}{2\omega_1}\right)^2\times\left[\frac{1}{3}\frac{\theta_1'''(0|\tau)}{\theta_1'(0|\tau)}-\frac{d^2}{dz^2}\ln\,\theta_1(z|\tau)\right], \quad (19)$$

where $z=\pi u/2\omega_1$ and $\tau=\omega_3/\omega_1$. In our case we have $\tau=i(\beta/2\pi)$ and $\omega_1=\pi/2$. Lamé's equation is extensively discussed for integer n. Also for positive half integers there exist some explicit solutions. For $n=-\frac{1}{2}$, however, there exists no explicit solution, at least to our knowledge. Of course there are some series expansions for general n too, but the recursion formulas for these coefficients are too complicated to be useful for our purposes.

Up to now we have discussed only the case where u^β is a symmetric function of x. Now we want to show that the function with the minimum uncertainty Δx is indeed symmetric. First assume that f^β is an arbitrary periodic function that is two times differentiable. Let us write $f^\beta(k)=r^\beta(k)e^{i\varphi^\beta(k)}$. Then we have

$$\langle x\rangle=\frac{i}{2\pi}\int_{-\pi}^{\pi}dk\,f^\beta(k)^*\frac{\partial}{\partial k}f^\beta(k)=-\frac{1}{2\pi}\int_{-\pi}^{\pi}dk[r^\beta(k)]^2\frac{\partial}{\partial k}\varphi^\beta(k), \quad (20)$$

$$\langle x^2\rangle=\frac{1}{4\beta}+\frac{1}{2\pi}\int_{-\pi}^{\pi}dk\left(\frac{\partial r^\beta(k)}{\partial k}\right)^2+\frac{1}{2\pi}\int_{-\pi}^{\pi}dk[r^\beta(k)]^2\left(\frac{\partial\varphi^\beta(k)}{\partial k}\right)^2+\frac{1}{8\pi}\int_{-\pi}^{\pi}dk[r^\beta(k)]^2\,\frac{\partial^2}{\partial k^2}\ln\,\theta_3\left(\frac{k}{2}\middle|\frac{i\beta}{2\pi}\right). \quad (21)$$

Thus the following inequality is valid:

$$(\Delta x)^2\geq\frac{1}{4\beta}+\frac{1}{2\pi}\int_{-\pi}^{\pi}dk\left(\frac{\partial r^\beta(k)}{\partial k}\right)^2+\frac{1}{8\pi}\int_{-\pi}^{\pi}dk[r^\beta(k)]^2\,\frac{\partial^2}{\partial k^2}\ln\,\theta_3\left(\frac{k}{2}\middle|\frac{i\beta}{2\pi}\right), \quad (22)$$

where the equality sign holds true if and only if $\partial\varphi^\beta(k)/\partial k$ is constant. In this case the periodicity of f^β implies that $\varphi^\beta(k)$ is of the form $\varphi^\beta(k)=kn+\varphi_0^\beta$, $n\in\mathbb{Z}$. Since the phase kn corresponds just to a shift by a lattice vector we may assume without any loss of generality that $f^\beta(k)=r^\beta(k)$ is a real function for the best localized ultralocalized function $u^\beta(k)$. It has to fulfill Eq. (17) and hence it has to be even. Thus the ultralocalized with minimal Δx is indeed symmetric with respect to a lattice point and in particular there is one that is symmetric with respect to the origin.

In terms of the coefficients $c_n^\beta=(1/2\pi)\int_{-\pi}^{\pi}e^{ikn}f^\beta(k)dk$ the expectation value $\langle x^2\rangle$ is given by the expression

$$\langle x^2\rangle=\frac{1}{4\beta}+\sum_{n=-\infty}^{\infty}|c_n^\beta|^2n^2+\sum_{m=-\infty}^{\infty}\sum_{n\neq 0}(c_m^\beta)^*c_{m+n}^\beta(-1)^n\frac{|n|}{8}\frac{1}{\sinh(\frac{\beta}{2}|n|)} \quad (23)$$

and the corresponding eigenvalue problem reads

$$c_n^\beta n^2+\frac{1}{4\beta}c_n^\beta+\sum_{m\neq 0}c_{m+n}^\beta(-1)^m\frac{|m|}{8}\frac{1}{\sinh(\frac{\beta}{2}|m|)}=\lambda^\beta c_n^\beta. \quad (24)$$

B. Anderson's ultralocalized functions

Since it is not possible to find an explicit expression for the exact solution of Eq. (17) or (24), we search for some approximations. For large β we use first-order perturbation theory: We use $H_0=-\partial^2/\partial k^2$ as the unperturbed operator with eigenvalues $\lambda_n^\infty=n^2$ and we treat $W^\beta=\frac{1}{4}(\partial^2/\partial k^2)\ln\,\theta_3(k/2\,|\,i\beta/2\pi)$ as a perturbation. Thus we get in first-order perturbation theory for the ground state

$$\lambda^\beta=\frac{1}{4\beta}+O(e^{-\beta}), \quad (25)$$

$$c_n^\beta=(-1)^{n+1}\frac{1}{8n}\frac{1}{\sinh\left(\frac{\beta}{2}n\right)}+O(e^{-\beta}),\quad n\neq 0 \tag{26}$$

$$c_0^\beta=1+O(e^{-\beta}). \tag{27}$$

In second-order perturbation theory we get the expression for the eigenvalue

$$\lambda^\beta=\frac{1}{4\beta}-\sum_{n=1}^{\infty}\frac{1}{32}\frac{1}{[\sinh(\frac{\beta}{2}n)]^2}+O(e^{-(3/2)\beta}). \tag{28}$$

Let us therefore discuss the ultralocalized function

$$c_n^\beta=\frac{d_n^\beta}{\|d^\beta\|},\quad \|d^\beta\|^2=\sum_{n=-\infty}^{\infty}|d_n^\beta|^2,$$

$$f^\beta(k)=\frac{g^\beta(k)}{\|g^\beta\|}, \tag{29}$$

$$\|g^\beta\|^2=\frac{1}{2\pi}\int_{-\pi}^{\pi}dk|g^\beta(k)|^2, \tag{30}$$

with

$$d_n^\beta=(-1)^{n+1}\frac{1}{8n}\frac{1}{\sinh\left(\frac{\beta}{2}n\right)},\quad n\neq 0 \tag{31}$$

$$d_0^\beta=1, \tag{32}$$

$$g^\beta(k)=\sum_{n=-\infty}^{\infty}d_n^\beta e^{-ikn}. \tag{33}$$

Note that this is Anderson's ultralocalized function since we have $d_n^\beta=-\langle W_n^\beta,x^2W_0^\beta\rangle/n^2$. This can be easily checked by using Eq. (13) and inserting the Fourier expansion of $\ln\theta_3$.

We can express $g^\beta(k)$ in terms of θ functions:

$$g^\beta(k)=1+\frac{1}{4}\ln\,\theta_3\left(\frac{k}{2}\middle|\frac{i\beta}{2\pi}\right)-\frac{1}{12}\ln\,\theta_1'\left(0\middle|\frac{i\beta}{2\pi}\right)+\frac{1}{12}\ln 2-\frac{\beta}{96}. \tag{34}$$

The formula for $\langle x^2\rangle$ now reads [use Eq. (23) to derive it]

$$\langle x^2\rangle=\frac{1}{4\beta}-\left(\frac{1}{32}\sum_{n=1}^{\infty}\frac{1}{[\sinh(\frac{\beta}{2}n)]^2}+2^{-9}{\sum_{n,m}}'\frac{1}{n+m}\times\frac{1}{\sinh[\frac{\beta}{2}(n+m)]}\frac{1}{\sinh(\frac{\beta}{2}m)}\frac{1}{\sinh(\frac{\beta}{2}n)}\right)\times\left(1+\sum_{n\neq 0}\frac{1}{n^2}\frac{1}{[\sinh(\frac{\beta}{2}n)]^2}\right)^{-1}, \tag{35}$$

where $\Sigma'_{n,m}$ means that the terms with $n=0, m=0$, and $m+n=0$ are excluded from the sum. Note that the term $-\Sigma'_{n,m}$ is positive and hence we have

$$\langle x^2\rangle>\frac{1}{4\beta}-\frac{1}{32}\sum_{n=1}^{\infty}\frac{1}{[\sinh(\frac{\beta}{2}n)]^2} \tag{36}$$

for this particular choice of f^β. Note also that $-\Sigma'_{n,m}$ is of $O(\beta^{-3})$ for $\beta\to 0$ and thus there is an additional positive contribution of $O(\beta^{-1})$ to the expectation value $\langle x^2\rangle$. Hence, for sufficiently small β the corresponding Anderson function is less localized than the corresponding Wannier functions and thus it cannot be called ultralocalized for these values of β.

In the case of large β we get the simple expression

$$\langle x^2\rangle=\frac{1}{4\beta}-\frac{1}{32}\frac{1}{(\sinh\frac{\beta}{2})^2}+O(e^{-(3/2)\beta}). \tag{37}$$

The ultralocalized functions read

$$u^\beta(x)=W_0^\beta+\frac{e^{-\beta/2}}{4}(W_1^\beta+W_{-1}^\beta)+O(e^{-\beta})=\left(\frac{2\beta}{\pi}\right)^{1/4}\left[e^{-\beta x^2}-\frac{e^{-\beta/2}}{4}(e^{-\beta(x+1)^2}+e^{-\beta(x-1)^2})\right]+O(e^{-\beta}). \tag{38}$$

Note that the oscillations of $u^\beta(x)$ are just half in height of the oscillations of the corresponding Wannier functions, which read in the same approximation

$$W_0^\beta(x)=\left(\frac{2\beta}{\pi}\right)^{1/4}\left(e^{-\beta x^2}-\frac{e^{-\beta/2}}{2}(e^{-\beta(x+1)^2}+e^{-\beta(x-1)^2})\right)+O(e^{-\beta}). \tag{39}$$

We have already mentioned that for sufficiently small β Anderson's ultralocalized functions are no longer ultralocalized ones. This can be seen explicitly if one calculates the limit $\beta\to 0$:

$$g^\beta(k)=1-\frac{k^2}{8\beta}+\frac{1}{4}\ln\,\theta_3\left(\frac{i\pi k}{\beta}\middle|\frac{2\pi i}{\beta}\right)-\frac{1}{12}\ln\,\theta_1'\left(0\middle|\frac{2\pi i}{\beta}\right)+\frac{1}{12}\ln 2-\frac{\beta}{96}. \tag{40}$$

In the limit $\beta\to 0$ we have

$$g^\beta(k)=-\frac{k^2}{8\beta}+\frac{\pi^2}{24\beta}+O(1) \tag{41}$$

and thus $f^0(k)$ is given by

$$f^0(k)=\sqrt{5}\left(\frac{1}{2}-\frac{3k^2}{2\pi^2}\right). \tag{42}$$

The corresponding "ultralocalized" function $u^0(x)$ reads

$$u^0(x)=\frac{1}{\sqrt{2\pi}}\int_{-\pi}^{\pi}dk\,f^0(k)\phi_k^0=\sqrt{5}\left(-\frac{\sin\pi x}{\pi x}-3\frac{\cos\pi x}{(\pi x)^2}+3\frac{\sin\pi x}{(\pi x)^3}\right). \tag{43}$$

It is easily seen that $\Delta x=\infty$ in this case. Note that $u^0(0)=0$, hence it less localized than the limit Wannier function[3] $W_0^0(x)=\sin\pi x/\pi x$ at the origin and in addition the oscilla-

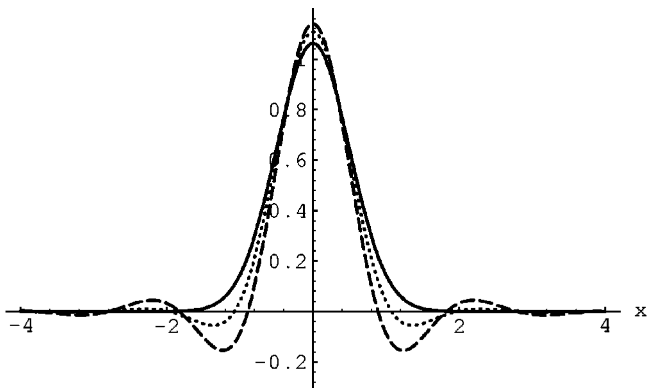

FIG. 1. Gauss function (solid curve), Wannier function (dashed curve), and Anderson's ultralocalized function (dotted curve) for $\beta=2$.

tions of $u^0(x)$ are larger than those of $W_0^0(x)$. Anderson's ultralocalized functions are shown in Figs. 1 and 2 for $\beta=2$ and 0.5, respectively. Numerical calculations yield that $\Delta x_{u^\beta}<1/4\beta$ is valid for approximately $\beta>0.5$.

C. Other kinds of ultralocalized functions for large β

We rewrite Eq. (17) as

$$-\frac{\partial^2 f^\beta(k)}{\partial k^2}+\left[\frac{1}{4\beta}+\frac{1}{\theta_3\left(\frac{k}{2}\middle|\frac{i\beta}{2\pi}\right)^{1/4}}\frac{\partial^2}{\partial k^2}\theta_3\left(\frac{k}{2}\middle|\frac{i\beta}{2\pi}\right)^{1/4}-\frac{1}{16}\left(\frac{\frac{\partial}{\partial k}\theta_3\left(\frac{k}{2}\middle|\frac{i\beta}{2\pi}\right)}{\theta_3\left(\frac{k}{2}\middle|\frac{i\beta}{2\pi}\right)}\right)^2\right]f^\beta(k)=\lambda^\beta f^\beta(k). \tag{44}$$

Note that

$$\frac{1}{\theta_3\left(\frac{k}{2}\middle|\frac{i\beta}{2\pi}\right)^{1/4}}\frac{\partial^2}{\partial k^2}\theta_3\left(\frac{k}{2}\middle|\frac{i\beta}{2\pi}\right)^{1/4}=O(e^{-\beta/2})$$

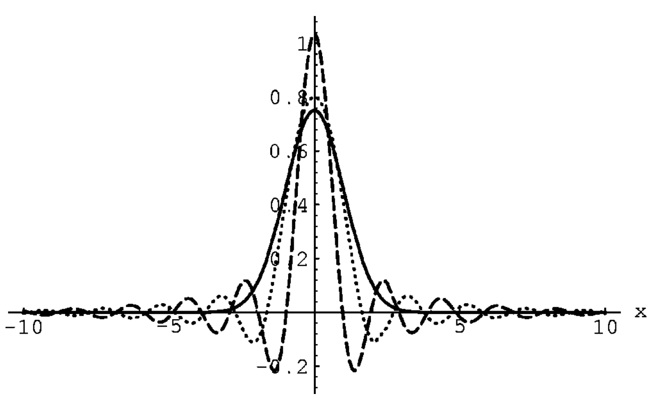

FIG. 2. Gauss function (solid curve), Wannier function (dashed curve), and Anderson's ultralocalized function (dotted curve) for $\beta=0.5$.

whereas

$$\left(\frac{\frac{\partial}{\partial k}\theta_3\left(\frac{k}{2}\middle|\frac{i\beta}{2\pi}\right)}{\theta_3\left(\frac{k}{2}\middle|\frac{i\beta}{2\pi}\right)}\right)^2=O(e^{-\beta}). \tag{45}$$

Thus the second term is much smaller than the first term. If we neglect the second term we get the equation

$$-\frac{\partial^2 f^\beta(k)}{\partial k^2}+\left[\frac{1}{4\beta}+\frac{1}{\theta_3\left(\frac{k}{2}\middle|\frac{i\beta}{2\pi}\right)^{1/4}}\times\frac{\partial^2}{\partial k^2}\theta_3\left(\frac{k}{2}\middle|\frac{i\beta}{2\pi}\right)^{1/4}\right]f^\beta(k)=\lambda^\beta f^\beta(k). \tag{46}$$

One immediately sees that $\lambda^\beta=1/4\beta$ is an eigenvalue whose corresponding eigenfunction is given by

$$f^\beta(k)=n^\beta\theta_3\left(\frac{k}{2}\middle|\frac{i\beta}{2\pi}\right)^{1/4}, \tag{47}$$

where n^β is the normalization constant. In fact, this is the ground state of Eq. (46), i.e., $\lambda^\beta=1/4\beta$ is the smallest eigenvalue of Eq. (46), which follows from the fact that the eigenfunction $f^\beta(k)=n^\beta\theta_3(k/2\,|\,i\beta/2\pi)^{1/4}$ has no zero (on the real line). The corresponding ultralocalized function is again denoted by $u^\beta(x)$. In first-order perturbation we obtain

$$\lambda^\beta=\langle x^2\rangle_{u^\beta}=\frac{1}{4\beta}-\frac{1}{32\pi}\int_{-\pi}^{\pi}dk(n^\beta)^2\frac{\left[\frac{\partial}{\partial k}\theta_3\left(\frac{k}{2}\middle|\frac{i\beta}{2\pi}\right)\right]^2}{\theta_3\left(\frac{k}{2}\middle|\frac{i\beta}{2\pi}\right)^{3/2}}. \tag{48}$$

Using partial integration and the differential equation for the θ function we arrive at

$$\langle x^2\rangle_{u^\beta}=\frac{1}{4\beta}-\frac{1}{2}\frac{\partial}{\partial\beta}\ln\left[\frac{1}{2\pi}\int_{-\pi}^{\pi}dk\;\theta_3\left(\frac{k}{2}\middle|\frac{i\beta}{2\pi}\right)^{1/2}\right] \tag{49}$$

$$=\frac{1}{8\beta}-\frac{1}{2}\frac{\partial}{\partial\beta}\times\ln\left[\sqrt{\frac{\pi}{4\beta}}\int_{-\pi}^{\pi}dk\;e^{-k^2/4\beta}\theta_3\left(\frac{i\pi k}{\beta}\middle|\frac{2\pi i}{\beta}\right)^{1/2}\right]. \tag{50}$$

For large and small values of β we have the approximations

$$\langle x^2\rangle_{u^\beta}=\frac{1}{4\beta}-\frac{1}{8}e^{-\beta}+O(e^{-2\beta})\quad\text{for large}\quad\beta, \tag{51}$$

$$\langle x^2\rangle_{u^\beta}=\frac{1}{8\beta}+O(\beta^{-3/2}e^{-\pi^2/4\beta})\quad\text{for small}\quad\beta. \tag{52}$$

Hence these functions are ultralocalized not only for large β but also for small β. For large β the ultralocalized functions are given by

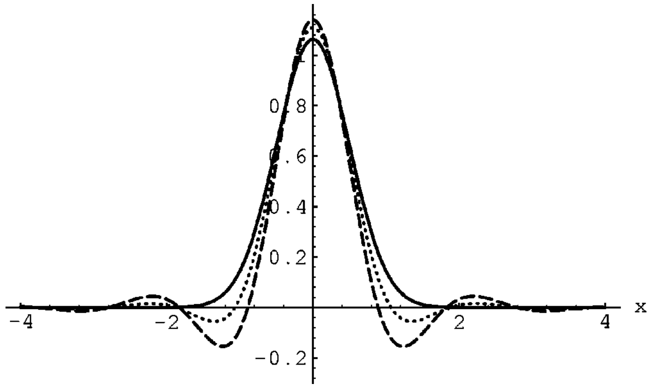

FIG. 3. Gauss function (solid curve), Wannier function (dashed curve), and ultralocalized function (dotted curve) for $\beta=2$.

$$u^{\beta}(x)=\left(\frac{2\beta}{\pi}\right)^{1/4}\left[e^{-\beta x^2}-\frac{e^{-\beta/2}}{4}(e^{-\beta(x+1)^2}+e^{-\beta(x-1)^2})\right] +O(e^{-\beta}). \tag{53}$$

Note that this is the same as Anderson's function, which also follows from the fact that both ultralocalized functions are exact solutions of Eq. (17) up to $O(e^{-\beta})$. The ultralocalized function is shown for $\beta=2$ in Fig. 3. Compare it with Anderson's ultralocalized function in Fig. 1.

It is also possible to calculate an approximation for small β. The ultralocalized functions read

$$u^{\beta}(x)=\left(\frac{4\beta}{\pi}\right)^{1/4}e^{-2\beta x^2}+O(\beta^{3/4}e^{-\pi^2/8\beta}). \tag{54}$$

However, we have to stress that $u^{\beta}(x)$ decreases only exponentially, i.e., $|u^{\beta}(x)|<A^{\beta}e^{-(\beta/2)|x|}$, which is due to the term of $O(\beta^{3/4}e^{-\pi^2/8\beta})$. The $L^2(\mathbb{R})$ norm of this term is of $O(e^{-\pi^2/8\beta})$. Note that the parameter β has been ''doubled,'' i.e., we have started with a Gaussian $e^{-\beta x^2}$ and ended up with a ultralocalized function $u^{\beta}(x)$ that is approximately a Gaussian $e^{-2\beta x^2}$. See Fig. 4, which shows the ultralocalized function for $\beta=0.5$.

Note also that all the ultralocalized functions that we have discussed so far fall off exponentially at infinity, namely, $|u^{\beta}(x)|\leq e^{-\beta/2}A^{\beta}$. This is due to the fact that $f^{\beta}(k)$ is analytic for $|\mathrm{Im}\,k|\leq\beta/2$ in all these cases.

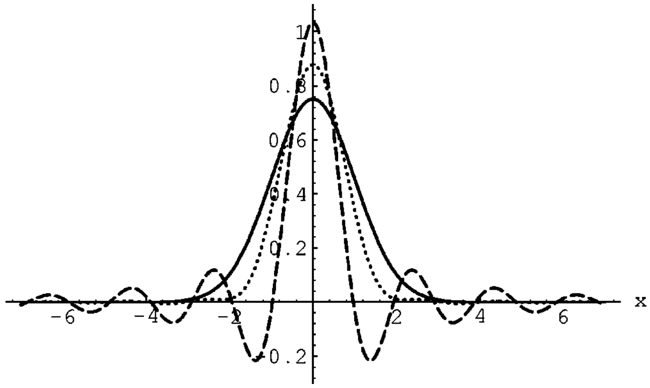

FIG. 4. Gauss function (solid curve), Wannier function (dashed curve), and ultralocalized function (dotted curve) for $\beta=0.5$.

D. An ultralocalized function for small β

So far we have mainly discussed approximations of Eq. (17) for large β. Now we want to discuss also ultralocalized functions for small β. To this end we first discuss the case $\beta=0$, which can be solved exactly. If one tries to calculate the limit $\beta\to 0$ of Eq. (17), one encounters the following problem: The expression

$$\begin{aligned}\frac{1}{4\beta}+\frac{1}{4}\frac{\partial^2}{\partial k^2}\ln\,\theta_3\left(\frac{k}{2}\middle|\frac{i\beta}{2\pi}\right) &=\frac{1}{4\beta}+\frac{1}{4}\frac{\partial^2}{\partial k^2}\ln\left[e^{-k^2/2\beta}\theta_3\left(\frac{i\pi}{\beta}k\middle|\frac{2i\pi}{\beta}\right)\right]\\ &=\frac{1}{4}\frac{\partial^2}{\partial k^2}\ln\,\theta_3\left(\frac{i\pi}{\beta}k\middle|\frac{2i\pi}{\beta}\right)\end{aligned} \tag{55}$$

''converges'' to ''$(1/0)\Sigma_{n=-\infty}^{\infty}\delta(k-2\pi n)$.'' Thus we calculate $\langle x^2\rangle$ for $u^0(x)$ directly. We have

$$u^0(x)=\frac{1}{2\pi}\int_{-\pi}^{\pi}dk\ f^0(k)e^{ikx}. \tag{56}$$

Since at least $xu^0(x)$ has to be square integrable, we require that $f^0(k)$ is absolutely continuous and $f^0(\pm\pi)=0$. Thus

$$\begin{aligned}xu^0(x)&=\frac{-i}{2\pi}\int_{-\pi}^{\pi}dk\ f^0(k)\ \frac{\partial}{\partial k}e^{ikx}\\ &=\frac{i}{2\pi}\int_{-\pi}^{\pi}dk\ \frac{d}{dk}f^0(k)e^{ikx}\end{aligned} \tag{57}$$

and hence

$$\langle x^2\rangle=\langle xu^0,xu^0\rangle=\frac{1}{2\pi}\int_{-\pi}^{\pi}dk\left|\frac{d}{dk}f^0(k)\right|^2 \tag{58}$$

has to be minimized with the constraint $(1/2\pi)\int_{-\pi}^{\pi}dk|f^0(k)|^2=1$ and the boundary conditions $f^0(\pm\pi)=0$. The corresponding Euler-Lagrange equation

$$\frac{d^2}{dk^2}f^0(k)+\lambda^0f^0(k)=0 \tag{59}$$

can be solved immediately and we obtain

$$f^0(k)=\sqrt{2}\ \cos\frac{k}{2},\quad \lambda^0=\frac{1}{4}. \tag{60}$$

It seems as if it were necessary to assume that $(d^2/dk^2)\,f^0(k)$ exists, but one can prove that the function $f^0(k)$ that minimizes Eq. (58) is two times differentiable.

The corresponding ultralocalized function reads

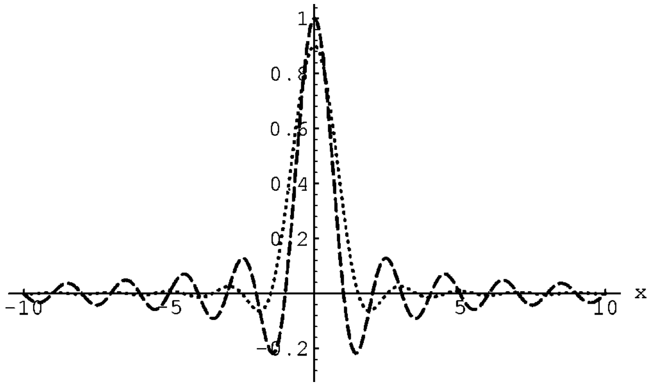

FIG. 5. Wannier function (dashed curve) and ultralocalized function (dotted curve) for $\beta=0$.

$$u^0(x)=\frac{1}{2\pi}\int_{-\pi}^{\pi}dk\sqrt{2}\cos\frac{k}{2}e^{ikx}$$
$$=\frac{\sqrt{2}}{2\pi}\left(\frac{\sin\pi\left(x+\frac{1}{2}\right)}{x+\frac{1}{2}}-\frac{\sin\pi\left(x-\frac{1}{2}\right)}{x-\frac{1}{2}}\right)$$
$$=\frac{\sqrt{2}}{2\pi}\frac{\cos\pi x}{x^2-\frac{1}{4}} \tag{61}$$

and we have $\langle x^2\rangle=\frac{1}{4}$; see Fig. 5. Note that u^0 falls off as $1/x^2$ for $x\rightarrow\pm\infty$, whereas the corresponding Wannier functions fall off as $1/x$.

We are interested in ultralocalized functions not only for $\beta=0$ but also for small β. A possible approximation for small β is to take $f^\beta(k)=f^0(k)$, but this choice has the disadvantage that $f^0(k)$ is not differentiable at $k=\pm\pi$ if it is continued periodically. However, this would imply that the corresponding ultralocalized functions would not fall off exponentially. Hence we look for an analytic function $f^\beta(k)$, which gives $f^0(k)$ in the limit $\beta\rightarrow 0$. A function with these properties is

$$f^\beta(k)=\frac{g^\beta(k)}{\|g^\beta\|},$$
$$g^\beta(k)=\cos\frac{k}{2}\frac{\theta_2\left(\frac{k}{2}\middle|\frac{i\beta}{2\pi}\right)}{\theta_3\left(\frac{k}{2}\middle|\frac{i\beta}{2\pi}\right)}=\cos\frac{k}{2}\frac{\theta_4\left(\frac{i\pi}{\beta}k\middle|\frac{2i\pi}{\beta}\right)}{\theta_3\left(\frac{i\pi}{\beta}k\middle|\frac{2i\pi}{\beta}\right)}. \tag{62}$$

Note that this function has period 2π and that

$$\lim_{\beta\rightarrow 0}\frac{\theta_2\left(\frac{k}{2}\middle|\frac{i\beta}{2\pi}\right)}{\theta_3\left(\frac{k}{2}\middle|\frac{i\beta}{2\pi}\right)}=\begin{cases}1 & \text{if } k\in[2\pi n-\pi,2\pi n+\pi], n \text{ even}\\ -1 & \text{if } k\in[2\pi n-\pi,2\pi n+\pi], n \text{ odd.}\end{cases} \tag{63}$$

Here it seems rather heuristic to use this particular choice of $f^\beta(k)$, so we give another motivation for it. We expand $f^0(k)$ into a Fourier series. We have

$$\frac{1}{2\pi}\int_{-\pi}^{\pi}dk\, f^0(k)e^{ikn}=\frac{1}{2\pi}\int_{-\pi}^{\pi}dk\sqrt{2}\cos\frac{k}{2}e^{ikn}$$
$$=\frac{1}{\sqrt{2}\pi}(-1)^{n+1}\left(\frac{1}{n+\frac{1}{2}}-\frac{1}{n-\frac{1}{2}}\right)$$
$$=\frac{1}{\sqrt{2}\pi}(-1)^n\frac{1}{n^2-\frac{1}{4}} \tag{64}$$

and thus

$$f^0(k)=\frac{1}{\sqrt{2}\pi}\sum_{n=-\infty}^{\infty}(-1)^{n+1}\left(\frac{1}{n+\frac{1}{2}}-\frac{1}{n-\frac{1}{2}}\right)e^{ikn}$$
$$=\frac{1}{\sqrt{2}\pi}\sum_{n=-\infty}^{\infty}(-1)^n\frac{1}{n^2-\frac{1}{4}}e^{ikn}. \tag{65}$$

Now we choose

$$h^\beta(k)=\frac{1}{\sqrt{2}\pi}\sum_{n=-\infty}^{\infty}(-1)^{n+1}\times\left(\frac{\beta}{2\sinh\frac{\beta}{2}\left(n+\frac{1}{2}\right)}-\frac{\beta}{2\sinh\frac{\beta}{2}\left(n-\frac{1}{2}\right)}\right)e^{ikn}, \tag{66}$$

for which $\lim_{\beta\rightarrow 0}h^\beta(k)=f^0(k)$ is obvious. Then one can easily show that $h^\beta(k)$ is equal to $[\theta_2(k/2|i\beta/2\pi)/\theta_3(k/2|i\beta/2\pi)]\cos(k/2)$ up to a constant. Note that $\theta_2(k/2|i\beta/2\pi)/\theta_3(k/2|i\beta/2\pi)$ is a multiple of one of Jacobi's elliptic functions, namely, $\mathrm{cd}(u)$, where $u=(k/2)\,\theta_3(0|i\beta/2\pi)^2$, and the Fourier transforms of the Jacobian elliptic functions are well known.[7]

E. Other kinds of ultralocalized functions for small β

Here we consider a family of different ultralocalized functions. We choose $f^\beta(k)$ as

$$f_\alpha^\beta(k)=n_\alpha^\beta\theta_3\left(\frac{k}{2}\middle|\frac{i\beta}{2\pi}\right)^\alpha, \tag{67}$$

with

$$n_\alpha^\beta=\left(\frac{1}{2\pi}\int_{-\pi}^{\pi}dk\ \theta_3\left(\frac{k}{2}\middle|\frac{i\beta}{2\pi}\right)^{2\alpha}\right)^{-1/2}, \tag{68}$$

where α is a real parameter that is assumed to vary between 0 and $\frac{1}{2}$, respectively. Note that $\alpha=0$ gives the symmetric Wannier functions, whereas $\alpha=\frac{1}{4}$ corresponds to the ultralocalized functions of Sec. IV C, and the choice $\alpha=\frac{1}{2}$ yields the original Gaussian.

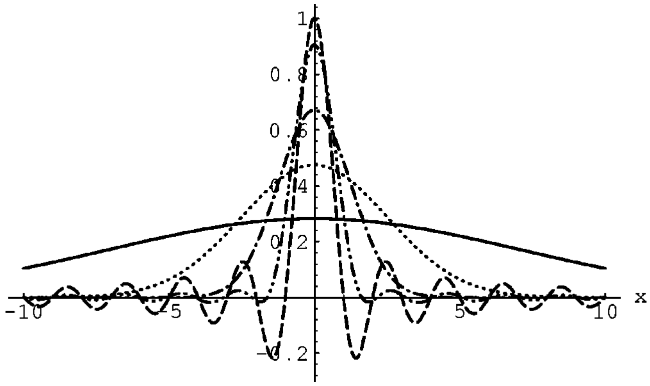

FIG. 6. Gauss function (solid curve), Wannier function (dashed curve), and the ultralocalized functions u_α^β for $\beta=0.01$ and $\alpha=\frac{1}{16}$ (dotted curve), $\alpha=\frac{1}{64}$ (dot-dashed curve), and $\alpha=\frac{1}{256}$ (double-dot–dashed curve).

The corresponding expectation values $\langle x^2\rangle_{u_\alpha^\beta}$ read

$$\langle x^2\rangle_{u_\alpha^\beta}=\frac{\alpha}{2\beta}-\frac{1}{2}\frac{\partial}{\partial\beta}\times\ln\left[\sqrt{\frac{\pi}{4\beta}}\int_{-\pi}^{\pi}dk\ e^{-\alpha k^2/\beta}\theta_3\left(\frac{i\pi k}{\beta}\middle|\frac{2\pi i}{\beta}\right)^{2\alpha}\right]. \tag{69}$$

For small and large values we get the approximations

$$\langle x^2\rangle_{u_\alpha^\beta}=\frac{1}{4\beta}-\alpha(1-2\alpha)e^{-\beta}+O(e^{-2\beta})\quad\text{for }\ \beta\to\infty, \tag{70}$$

$$\langle x^2\rangle_{u_\alpha^\beta}=\frac{\alpha}{2\beta}+O\left(\sqrt{\frac{\alpha}{\beta}}\left(\frac{1}{\beta}+\frac{1}{\alpha}\right)e^{-\alpha\pi^2/\beta}\right)\quad\text{for }\ \beta\to 0. \tag{71}$$

The ultralocalized functions read for large β

$$u_\alpha^\beta(x)=\left(\frac{2\beta}{\pi}\right)^{1/4}\left[e^{-\beta x^2}-\frac{1-2\alpha}{2}e^{-\beta/2}\times(e^{-\beta(x+1)^2}+e^{-\beta(x-1)^2})\right]+O(e^{-\beta}). \tag{72}$$

For small β the calculations are analogous to those of Sec. IV C:

$$u_\alpha^\beta(x)=\frac{1}{(2\pi)^{1/2}}\int_{-\pi}^{\pi}dk\ f_\alpha^\beta(k)\phi_k^\beta=\left(\frac{\beta}{\pi\alpha}\right)^{1/4}e^{-(\beta/2\alpha)x^2}+O\left(\left(\frac{\beta}{\alpha}\right)^{3/4}e^{-\alpha\pi^2/2\beta}\right). \tag{73}$$

Thus the ultralocalized function is the sum of a Gaussian and a small rest if β is sufficiently small. By an appropriate choice of α one can make the Gaussian fall off much faster than the original Gaussian. However, note that one cannot choose α arbitrarily small since the term of $O((\beta/\alpha)^{3/4}e^{-\alpha\pi^2/2\beta})$ is no longer small for too small values of α. More precisely, α can only be chosen such that $\alpha\gtrsim\beta$ if one wants an ultralocalized function that does not differ much from a Gaussian. These ultralocalized functions are shown for various values of α in Fig. 6.

V. CONCLUSION

We have studied the localization properties of Wannier functions composed of Gaussian orbitals and of corresponding ultralocalized functions. In particular, we have shown that the Wannier functions are better localized than the original Gauss functions near the origin, whereas the Gaussians fall off faster at infinity. Thus, it is possible to construct ultralocalized functions whose uncertainty Δx is smaller than the uncertainty Δx of the corresponding Wannier functions and the original Gaussians. We have proved that the ultralocalized functions that have the minimal uncertainty Δx can be found by solving Lamé's equations. Since this equation cannot be solved exactly, we have discussed several approximate solutions. One of these ultralocalized functions is very remarkable: If we start with a rather extended Gaussian $e^{-\beta x^2}$, where β is small, then we can construct an ultralocalized function that is the sum of a more localized Gaussian and a small rest, $e^{(-\beta/\alpha)x^2}+\varepsilon(x)$ with $\alpha<1$.

ACKNOWLEDGMENT

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