Variable-phase method and Levinson's theorem in two dimensions: Application to a screened Coulomb potential

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Abstract

The variable-phase approach is applied to scattering and bound states in an attractive Coulomb potential, statically screened by a two-dimensional (2D) electron gas. A 2D formulation of Levinson's theorem is used for bound-state counting and a hitherto undiscovered, simple relationship between the screening length and the number of bound states is found. As the screening length is increased, sets of bound states with differing quantum numbers appear degenerately.

73.20.Dx, 73.50.Bk, 03.65.Nk, 03.65.Ge

The quantum mechanics of low-dimensional systems has become a major research field with the advent of growth techniques for the realization of semiconductor quantum wells. Almost all of the computational techniques developed for three-dimensional (3D) problems have already been extended to lower dimensions. The variable-phase method for the calculation of the scattering phase shifts was introduced long ago by Morse and Allis [1] and expanded by Calogero [2], Babikov [3] and others [4] but has to our knowledge never been used for analysis of any realistic two-dimensional problem. In this Letter we use the variable-phase method to treat both scattering and bound states on the same footing for the Coulomb potential statically screened by 2D electron gas. This potential plays a central role in the physics of semiconductor heterostructures, one of the most rapidly growing fields in condensed matter physics. Despite having been studied for approximately 30 years [5,6] this potential exhibits some peculiar features which have never been noticed until now, e.g., as the screening length increases, sets of bound states with differing quantum numbers appear degenerately. These degeneracies are not, however, the same as the degeneracies in the unscreened spectrum. We also report a hitherto undiscovered, simple relationship connecting the number of bound states to the screening length.

In what follows we consider a simple case in which a screened charge resides in the same plane as a screening 2D electron gas. This geometry is appropriate to the problem of screened excitons [7] or impurities [6] in a narrow quantum well. We assume that an attractive potential is created by a point charge e at the origin and use throughout this paper excitonic Rydberg units where length and energy are scaled, respectively, by the effective Bohr radius a^* and Rydberg Ry^* . In these units and geometry the Thomas-Fermi expression for the statically screened potential in the electron plane [6,7] is

$$V_s(q) \;=\; -\,2\frac{2\pi}{q+q_s}\;, \tag{1}$$

where q_s is the 2D screening wavenumber. Eq. (1) is the 2D analogue of the Yukawa potential. Taking the 2D Fourier transformation of Eq. (1) yields in real space

$$V_s(\rho) \;=\; -\,2\left\{\frac{1}{\rho}-q_s\int_0^\infty \frac{J_0(q\rho)}{q+q_s}dq\right\}\;, \tag{2}$$

where $J_0(q\rho)$ is the Bessel function, and $\rho = (x^2 + y^2)^{1/2}$ is the in-plane distance from the origin.

To describe the application of the variable-phase method in 2D we consider a particle moving with energy $E = k^2$ in the potential $V(\rho)$ which has radial symmetry. Since the potential is symmetric, we can separate variables in the expression for the wave function:

$$\Psi(\rho, \varphi) \;=\; \sum_{m=0}^{\infty} R_m(\rho)\; \cos(m\varphi)\;, \tag{3}$$

where m is the absolute value of the projection of the angular momentum onto the symmetry axis of the potential. At large distances from the scattering center, the radial function satisfies the free Bessel equation, whose general solution is

$$\begin{aligned} R_m(\rho) \;&=\; A_m[J_m(k\rho)\cos\delta_m - N_m(k\rho)\sin\delta_m] \\ &\stackrel{\rho\to\infty}{\longrightarrow}\; A_m\left(\frac{2}{\pi k\rho}\right)^{1/2}\cos(k\rho - (2m+1)\pi/4 + \delta_m)\;, \end{aligned} \tag{4}$$

where δ_m is the scattering phase shift [6,8], $J_m(k\rho)$ and $N_m(k\rho)$ are the Bessel and Neumann functions, respectively. Both total and transport cross sections in 2D can be expressed via the scattering phase shifts in a simple fashion [6].

In the variable-phase method A_m and δ_m are considered not as constants but as functions of the distance ρ . The phase function $\delta_m(\rho)$ is the phase shift produced by a potential cut-off at a distance ρ. Then the scattering phase shift can be obtained as a large distance limit of the phase function $\delta_m(\rho)$, which satisfies the following first-order, non-linear differential equation originating from the radial Schrödinger equation [3]:

$$\frac{d}{d\rho}\delta_m(\rho) \;=\; -\frac{\pi}{2}\rho V(\rho)[J_m(k\rho)\cos\delta_m(\rho) - N_m(k\rho)\sin\delta_m(\rho)]^2 \tag{5}$$

with the boundary condition

$$\delta_m(0) \;=\; 0\;. \tag{6}$$

Eq. (6) ensures that the radial function does not diverge at $\rho = 0$. Physically one can view the phase function as measuring the retardation of the scattering wave function due to the

potential. From this view it is clear that Eq. (6) is the correct boundary condition since the potential can produce no retardation at the origin. The total scattering phase shift is given as an asymptote of $\delta_m(\rho)$:

$$\delta_m \;=\; \lim_{\rho\to\infty}\delta_m(\rho)\ . \tag{7}$$

For numerical convenience, instead of the boundary condition Eq. (6), the small-ρ expansion is used

$$\delta_m(\rho) \;\approx\; -\frac{\pi k^{2m}}{2^{2m+1}(m!)^2}\int_0^\rho V(\rho')\rho'^{2m+1}d\rho'\ , \quad \rho\;\to\;0\ . \tag{8}$$

It is also useful to rewrite Eq. (2) in terms of special functions [6,9] as

$$V_s(\rho) \;=\; -2\left\{\frac{1}{\rho}-\frac{\pi}{2}q_s[\mathbf{H}_0(q_s\rho)-N_0(q_s\rho)]\right\}\ , \tag{9}$$

where $\mathbf{H}_0(q_s\rho)$ and $N_0(q_s\rho)$ are the Struve and Neumann functions, respectively. Series representations of these functions for small values of argument and asymptotic expansions for large values of argument allow the accurate calculation of $V_s(\rho)$ for all values of $q_s\rho$. Asymptotic expressions for the potential are

$$V_s(\rho) \;\sim\; -\frac{2}{q_s^2\rho^3}\left\{1+\sum_{n=1}^{p}\;(-1)^n\;\frac{[(2n+1)!!]^2}{(q_s\rho)^{2n}}\;+\;O[(q_s\rho)^{-2p-2}]\;\right\}\ , \quad q_s\rho\;\gg\;1\ , \tag{10}$$

and

$$V_s(\rho) \;\sim\; -2[\rho^{-1}\;+\;q_s\ln(Cq_s\rho)]+O(q_s\rho)\ , \quad q_s\rho\;\ll\;1\ , \tag{11}$$

where $C=\frac{1}{2}\exp(\gamma)$, and γ is Euler's constant. The asymptotic expressions Eqs. (10,11) show that the potential $V_s(\rho)$ satisfies the conditions:

$$\int_\rho^\infty V(\rho')\;d\rho'\;\to\;0\ , \quad \rho\;\to\;\infty\ , \tag{12}$$

and

$$\rho^2V(\rho)\;\to\;0\ , \quad \rho\;\to\;0\ , \tag{13}$$

which are sufficient to allow application of the variable-phase method for this potential.

Figure 1 shows the k dependence of the phase shifts δ_m obtained by the numerical solution of Eq. (5) with the initial condition Eq. (8) for the screened Coulomb potential $V_s(\rho)$. The distinctive feature of this plot to which we draw attention is that in the low-energy limit, $k \to 0$, the scattering phase shift is an integer number of π :

$$\lim_{k\to 0} \delta_m \;=\; \nu\pi \;. \tag{14}$$

This behavior may be understood recalling Levinson's theorem [10] which connects the zero-energy scattering phase shift with the number of the bound states for non-relativistic particles in 3D. Recently Levinson's theorem has been discussed for Dirac particles, multichannel scattering, multi-particle single-channel scattering, one-dimensional scattering systems, systems with non-uniform effective mass, and even for time-periodic potentials [11]. However its applicability to the 2D scattering problem has not been considered yet. We expect that this fundamental theorem holds also in 2D in the form of Eq. (14), where ν is the number of bound states for a given m. A simple proof for $m \neq 0$ follows from Eq. (5) in the same fashion as Calogero's proof of Levinson's theorem in the 3D case [2]. For $m = 0$ the proof is more complicated due to the logarithmic divergence of the Neumann function, $N_0(k\rho)$. A rigorous proof of Levinson's theorem in 2D, based on analytic properties of the scattering matrix [13], is needed. We have, however, verified the validity of Eq. (14) for *all* m values in the analytically tractable case of a circular finite potential well [12].

Despite its appeal, Levinson's theorem has not been widely used to enumerate bound states since there exists an ambiguity in the usual definition of δ_m, being defined only up to $\mathrm{mod}(\pi)$ [14]. However using the variable phase approach avoids this problem since the phase function is uniquely defined by Eqs. (5,6) for all ρ.

In Fig. 2 the number of bound states, obtained as the low-energy limit of the scattering phase shift in units of π , is plotted as a function of the screening length $r_s = 1/q_s$ for the potential V_s . As the screening length increases, the potential supports more bound states and these new bound states appear at critical values of the screening length indicated by the steps. One can see from the location of these steps that the ν-th bound state for a given

m appears at the critical screening length, given by a simple formula

$$(r_s)_c \;=\; \frac{(2m+\nu-1)(2m+\nu)}{2}\;, \qquad \nu = 1, 2,\;\; \ldots\;. \tag{15}$$

This intriguingly simple relation has, to our knowledge, never been reported despite numerous calculations of the binding energy in the screened Coulomb potential, since conventional numerical methods for the binding energy calculation fail for extremely shallow energy levels. Note that for $m = 0$ the first bound state appears immediately at $(r_s)_c \;=\; 0$, corresponding to the fact that there is always at least one bound state in any symmetric 2D attractive potential. Using Eq. (15) we can simply evaluate how many bound states the 2D statically-screened Coulomb potential will support for any value of m.

The Bargmann bound condition [15] re-stated for two dimensions [6] is $m\nu < r_s$. This gives a gross over-estimation of the number of the bound states; e.g., for $r_s = 4,\; m = 1$ this implies only that there are less than four bound states whereas there is in fact only one. In this sense the Bargmann condition is of limited utility.

For many applications (e.g., in a partition function calculation) the value of the binding energy, not just the number of bound states, is important. The variable-phase method provides an elegant and efficient solution of the eigenvalue problem as well. To approach this problem we recall that for the states with negative energy the wavenumber k is imaginary, $k = i\kappa$, and we introduce the function $\mu_m(\rho, \kappa)$ vanishing in the origin and satisfying a non-linear equation [3]

$$\frac{d}{d\rho}\mu_m(\rho,\kappa) \;=\; -\frac{\pi}{2}\rho V(\rho)\left[I_m(\kappa\rho)\cos\mu_m(\rho,\kappa) + \frac{2}{\pi}K_m(\kappa\rho)\sin\mu_m(\rho,\kappa)\right]^2\;, \tag{16}$$

where $I_m(\kappa\rho)$ and $K_m(\kappa\rho)$ are the modified Bessel functions of the first and second kind, respectively. The functions $I_m(\kappa\rho)$ and $K_m(\kappa\rho)$ represent two linearly independent solutions of the free radial-wave Schrödinger equation for the negative value of energy, $E = -\kappa^2$, and $\cot\mu_m$ characterizes the weights of the diverging (I_m) and converging (K_m) solutions as $\rho \to \infty$. For the bound state, the diverging solution vanishes, implying the asymptotic condition

$$\mu_m(\rho \to \infty \, , \kappa_\nu) \;=\; (\nu - 1/2)\pi \;, \qquad \nu = 1, 2, \;\; \ldots \;\; . \tag{17}$$

Here ν numerates the bound states for a given m and $(\nu - 1)$ is the number of non-zero nodes of the radial wave function. For numerical solution of Eq. (16) instead of the boundary condition $\mu_m(0, \kappa) = 0$ an approximate initial condition (analogous to the condition Eq. (8) for the phase function $\delta_m(\rho)$) is used.

The bound-state energies $E_{m,\nu}$ versus the screening length r_s for the potential V_s are plotted in Fig. 3. For clarity all the curves are normalized by the values of the energy for the unscreened potential [16], $E_{m,\nu}(q_s = 0) = -(\nu + m - 1/2)^{-2} = -(n + 1/2)^{-2}$. The principal quantum number n is given by $n = \nu + m - 1$. We note that the unscreened eigenstates with the same value of $m + \nu$ are degenerate. A consequence of the relationship in Eq. (15) is that when the bound states first appear (at $r_s = (r_s)_c$), eigenstates with the same value of $2m + \nu$ are degenerate. With increasing r_s this degeneracy is lifted and the degeneracy for the states with the same values of n appears as $r_s \to \infty$.

In conclusion, we have used the variable-phase method to study scattering and bound states in two dimensions. The 2D analogy of Levinson's theorem is formulated and verified empirically. A hitherto undiscovered, simple relationship between the screening length and the number of bound states in the statically-screened Coulomb potential has been found. Challenging problems such as a general proof of Levinson's theorem in 2D and the analytic derivation of Eq. (15) are clearly the subject of further research.

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FIGURES

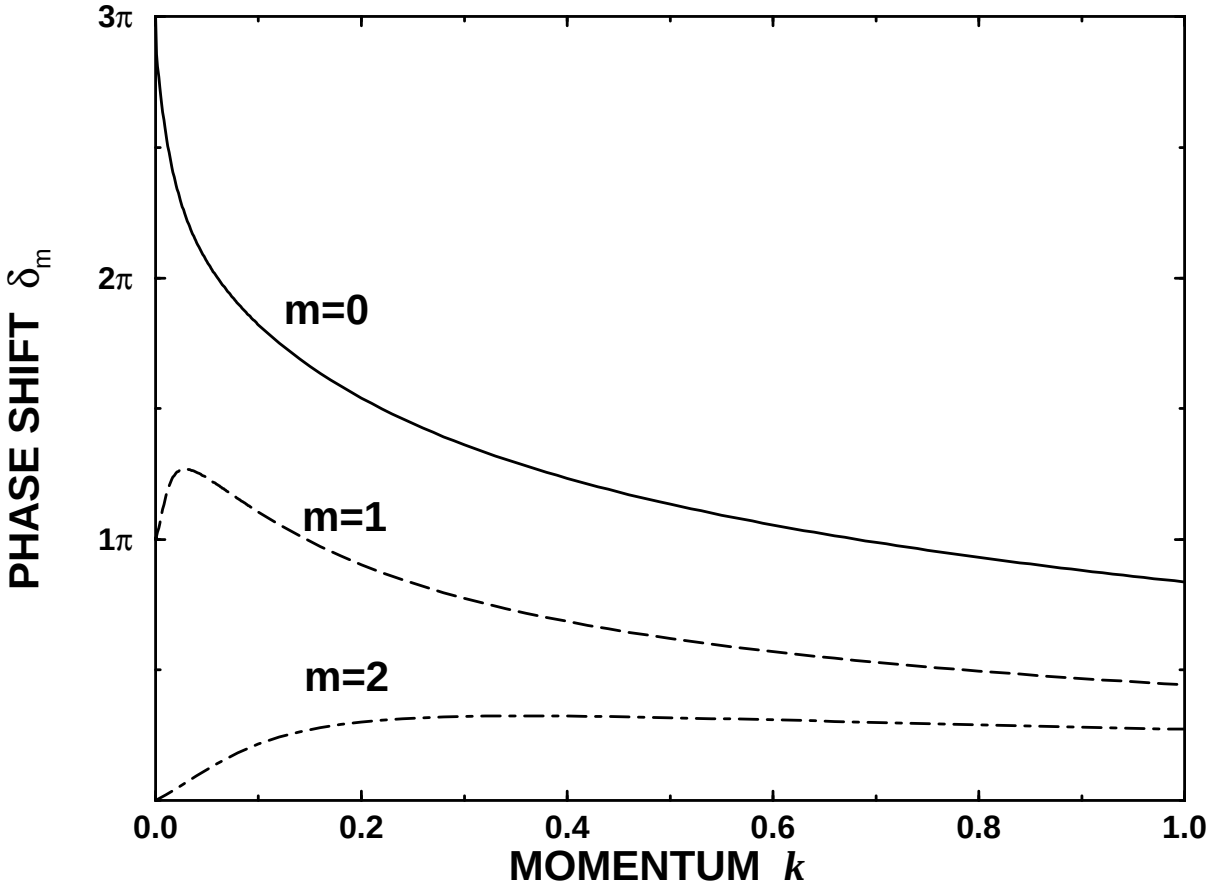

FIG. 1. Scattering phase shifts versus in-plane wave vector k (in units of inverse Bohr radius $1/a^*$) for a 2D particle in an attractive Coulomb potential screened by a 2D electron gas, screening length $r_s = 1/q_s = 5a^*$. Numbers show m values.

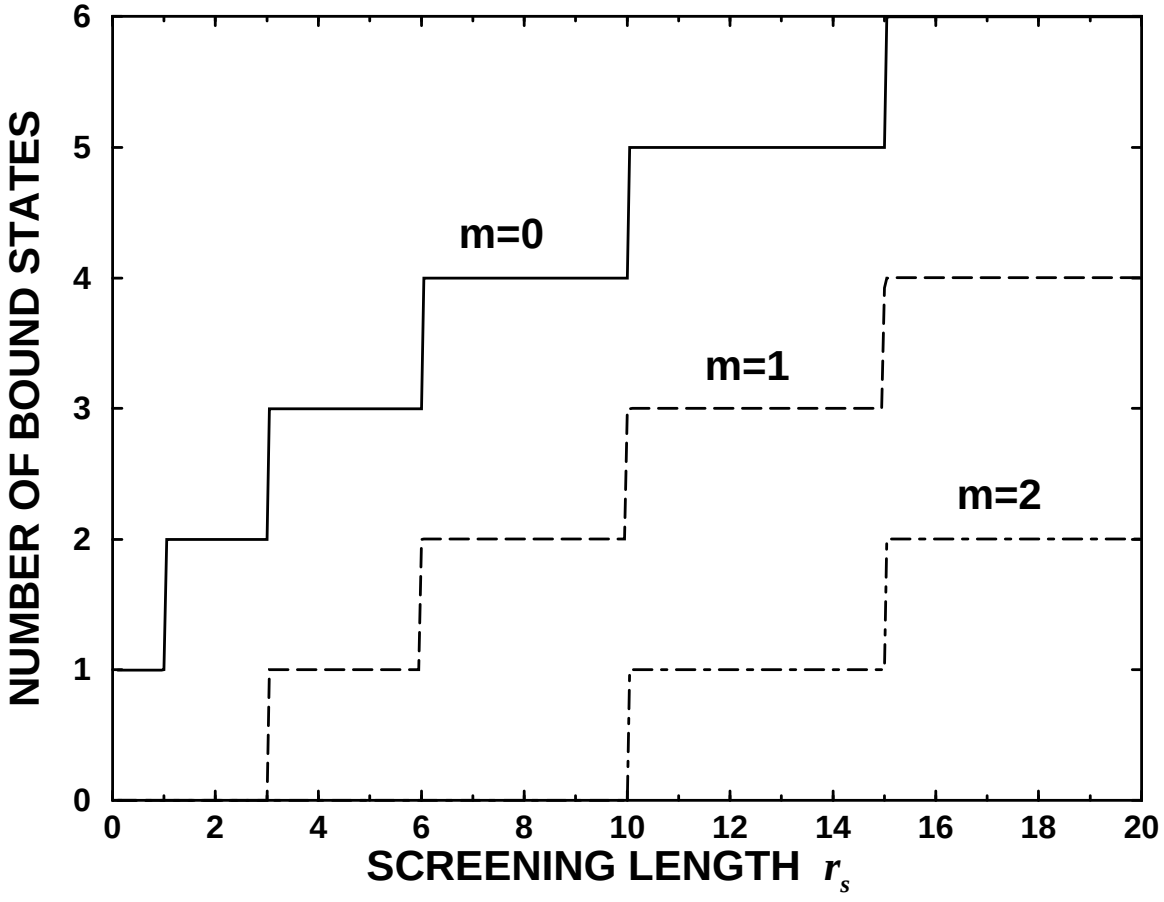

FIG. 2. Number of bound states, calculated as the low-energy limit of the phase shift, plotted versus the screening length r_s (in the units of Bohr radius a^*). The solid line corresponds to $m = 0$; dashed line, $m = 1$; dashed-dotted line, $m = 2$. New steps appear at $(r_s)_c = (2m + \nu - 1)(2m + \nu)/2$, $\nu = 1, 2, \ldots$.

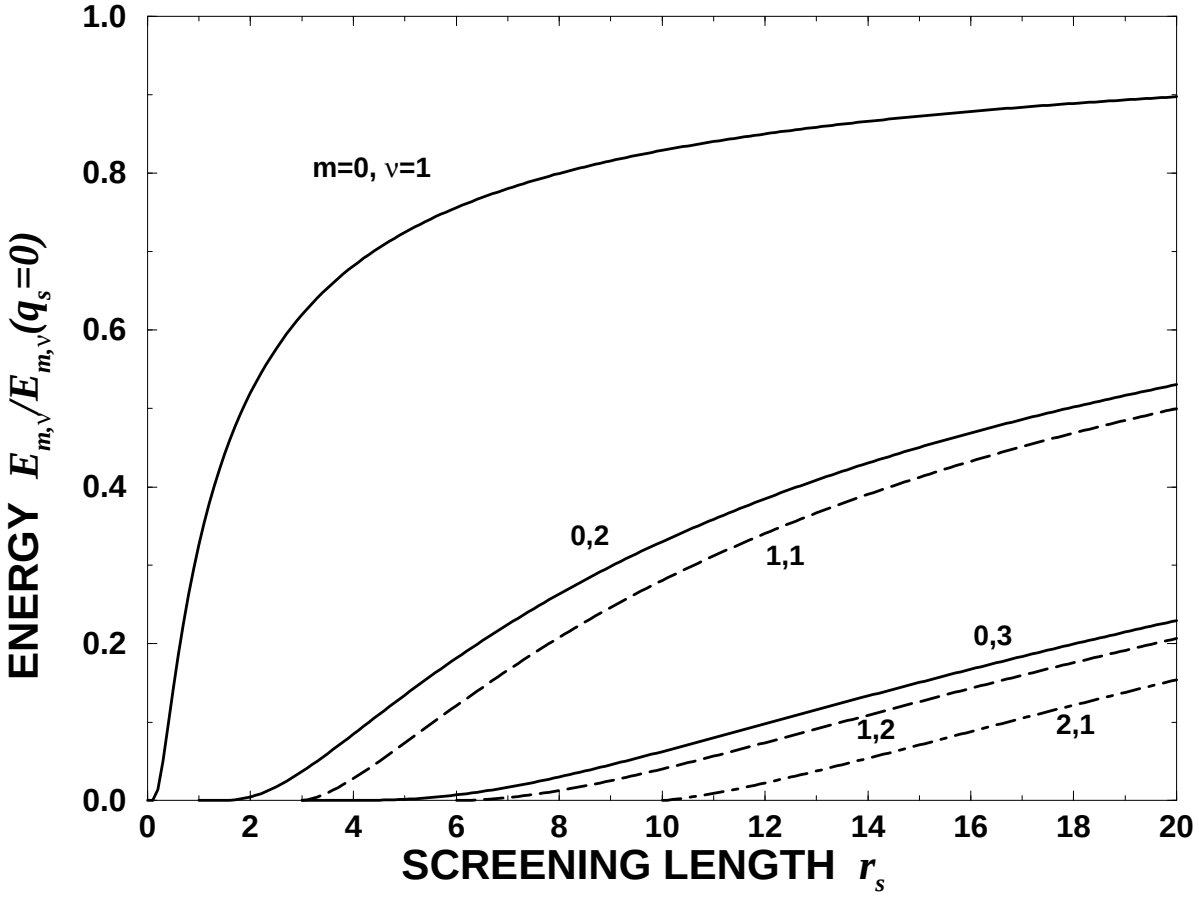

FIG. 3. The bound-state energies $E_{m,\nu}$ plotted versus the screening length r_s for different m values. The curves are normalized by the energies for the unscreened potential, $E_{m,\nu}(q_s = 0) = -(m + \nu - 1/2)^{-2}$. Numbers show m and ν values.