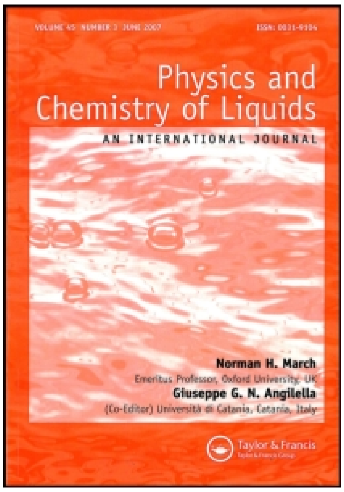

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Feynman propagator, density matrices and Green functions for the inhomogeneous electron liquid generated by a bare Coulomb potential in two dimensions

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For a two-dimensional homogeneous electron gas, the canonical density matrix $C(\mathbf{r}, \mathbf{r}'; \beta)$ is well-known. This object is related to the Feynman propagator $K(\mathbf{r}, \mathbf{r}'; t)$, where t is the time, by the transform $\beta \to \mathrm{i}t$. From the free electron form of $C(\mathbf{r}, \mathbf{r}'; \beta)$, the Green function follows in terms of the Bessel function K_0. When a bare Coulomb potential $-Ze^2/r$ is now 'switched on', one known property is the local density of states at the nucleus. This enables the imaginary part $\mathrm{Im}\, G$ of the Green function at the nucleus to be determined as an explicit function of energy E and nuclear charge Ze. Off-diagonal information on $\mathrm{Im}\, G$ will yield the real part of the Green function by using the Kramers–Krönig relation. The analysis of the two-dimensional Green function G into partial waves characterized by angular momentum quantum number ℓ is then considered. The imaginary part of G for $\ell = 0$ is determined in terms of a hypergeometric function. The real part is again in principle accessible by invoking the Kramers–Krönig relation. From the relation between G and the Laplace transform of C with respect to β, information is also obtained on the $\ell = 0$ partial wave component of the Slater sum $S(r, \beta) = C(\mathbf{r}, \mathbf{r}; \beta)$ and hence the Feynman propagator on the diagonal, in the limiting case $Z \to 0$.

Keywords: Inhomogeneous electron liquid; Two-dimensional Coulomb potential; Density matrices

PACS numbers: 05.30.Fk; 71.10.Ca; 31.15.Ew; 31.15.Bs

1. Introduction

A great deal of attention has been devoted to propagators generated by the bare Coulomb potential $-Ze^2/r$ in three dimensions. Thus, the Feynman propagator $K(\mathbf{r}, \mathbf{r}'; t)$, where t is the time, has been given by Blinder [1] in the form of an infinite

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series, which, however, remains complicated in that this result contains a variety of special functions including Whittaker functions, together with Laguerre and Hermite polynomials.

Here, therefore, we shall consider a related quantity, the canonical density matrix $C(\mathbf{r},\mathbf{r}';\beta)$, which is related to $K(\mathbf{r},\mathbf{r}';t)$ by the transformation $\beta\to it$ [1], along with the Dirac density matrix $\gamma(\mathbf{r},\mathbf{r}')$, but in what proves to be the mathematically simpler case of the same potential $-Ze^2/r$, but now in two dimensions. The canonical density matrix satisfies the Bloch equation [2]

$$\mathscr{H}_{\mathbf{r}}C(\mathbf{r},\mathbf{r}';\beta)=-\frac{\partial C(\mathbf{r},\mathbf{r}';\beta)}{\partial\beta},\tag{1}$$

where the now two-dimensional (2D) Hamiltonian $\mathscr{H}_{\mathbf{r}}$ has the explicit form

$$\mathscr{H}_{\mathbf{r}}=-\frac{\hbar^2}{2m}\nabla_{\mathbf{r}}^2-\frac{Ze^2}{r}\tag{2}$$

throughout the present study. The boundary condition to be combined with equation (1) is that $C(\mathbf{r},\mathbf{r}';0)=\delta(\mathbf{r}-\mathbf{r}')$.

In the limit $Z\to 0$, the free-particle canonical density matrix takes the well-known form in two dimensions

$$C_0(\mathbf{r},\mathbf{r}';\beta)=\frac{1}{2\pi\beta}\exp\left(\frac{-|\mathbf{r}-\mathbf{r}'|^2}{2\beta}\right),\tag{3}$$

going back to the celebrated study of Sondheimer and Wilson [3]. It is known that C and the Green function G are related via

$$\mathscr{L}_\beta\, C(\mathbf{r},\mathbf{r}';\beta)=G(\mathbf{r},\mathbf{r}';-E)\tag{4}$$

and inserting in equation (4) the free-particle result (3) we readily obtain the free-particle Green function in two dimensions as

$$G_0(\mathbf{r},\mathbf{r}';-E)=\frac{1}{\pi}\;K_0(\sqrt{2E}\;|\mathbf{r}-\mathbf{r}'|),\tag{5}$$

where $K_0(z)$ denotes the modified Bessel function.

It is relevant here to note, concerning the simplicity of the above 2D case, that when equation (3) is decomposed into 'partial waves' characterized by the angular momentum quantum number ℓ, the resulting ℓ-component $\mathscr{L}_\beta C_{0\ell}(r,r';\beta)$ takes the factorized form

$$\mathscr{L}_\beta\, C_{0\ell}(r,r';\beta)=f_\ell(r;E)\,f_\ell(r';E),\tag{6}$$

whereas March and Murray [4] in early work showed that for 3D the corresponding free-particle limit of $C_{0\ell}(r, r'; \beta)$ had the nonfactorizable form proportional to

$$\exp\left(-\frac{r^2 + r'2}{2\beta}\right)\frac{I_{\ell+(1/2)}(rr'/\beta)}{\sqrt{rr'}},$$

where $I_n(x)$ is the modified Bessel function $(-\mathrm{i})^n J_n(-\mathrm{i}x)$. We shall stress in section 2 below that the factorization property exhibited in equation (6) for the free-particle limit $Z \to 0$ in equations (1) and (2) continues to hold in the 2D Coulomb problem, which is the main focus of the present study. Continuing the outline of this article, section 3 moves from the canonical matrix discussed earlier to the Dirac density matrix $\gamma(\mathbf{r}, \mathbf{r}')$. As utilized by March and Murray, provided a constant greater than the lowest bound state eigenvalue is added, to bring the entire level spectrum in the energy range $0 < E < \infty$, $\gamma(\mathbf{r}, \mathbf{r}'; E)$ and $C(\mathbf{r}, \mathbf{r}'; \beta)$ are related by

$$C(\mathbf{r}, \mathbf{r}'; \beta) = \beta \int_0^\infty \gamma(\mathbf{r}, \mathbf{r}'; E) \exp(-\beta E) \mathrm{d}E. \tag{7}$$

Some results on the Dirac matrix $\gamma(\mathbf{r}, \mathbf{r}'; E)$ form the essence of section 3. Since it is known that the imaginary part of the Green function is directly related to $\partial\gamma(\mathbf{r}, \mathbf{r}'; E)/\partial E$, some discussion of the 2D Green function provides the focus of section 4. The article concludes with a summary, plus some proposals for future directions that should prove fruitful, in section 5.

2. The partial wave canonical density matrix in the 2D bare Coulomb case

The normalized wave functions $\psi_{n\ell}(\mathbf{r})$ generated by the bare Coulomb potential $-Ze^2/r$ in 2D take the explicit form in plane polar coordinates (r, θ), with $E_n = -k_{0n}^2$ say, and $Z = 1$ for simplicity,

$$\psi_{n\ell}(\mathbf{r}) = \left(\frac{k_{0n}^3 (n - |\ell|)!}{\pi(n + |\ell|)!}\right)^{1/2} (2k_{0n}r)^{|\ell|} \exp(-k_{0n}r) L_{n-|\ell|}^{2|\ell|}(2k_{0n}r) \exp(i\ell\theta). \tag{8}$$

The bound-state energy levels are given in 2D by

$$E_n = -\frac{1}{(n + (1/2))^2}. \tag{9}$$

The bound state (b) canonical density matrix $C^{(b)}(\mathbf{r}, \mathbf{r}'; \beta)$ written in terms of E_n and $\psi_{n\ell}$, reads

$$\begin{aligned} C_\ell^{(b)}(r, r'; \beta) = \sum_n \left(\frac{k_{0n}^3 (n - |\ell|)!}{\pi(n + |\ell|)!}\right) (2k_{0n}r)^{|\ell|} \exp(-k_{0n}r) L_{n-|\ell|}^{2|\ell|}(2k_{0n}r) \\ \times (2k_{0n}r')^{|\ell|} \exp(-k_{0n}r') L_{n-|\ell|}^{2|\ell|}(2k_{0n}r') \mathrm{e}^{\beta/(n+(1/2))^2}. \end{aligned} \tag{10}$$

Turning from this wave function form of $C_\ell^{(b)}$ to direct Green function results, prompted by the relation (4), we seek the partial wave component of G for the 2D bare Coulomb potential. One place, among others, where this is conveniently given, is in the study of Inomata [5]. His equation (26) corresponds to (in atomic units $m = \hbar = 1$, which we use here)

$$G_\ell(r, r'; E) = \frac{2i^{\ell-2}\Gamma(p + \ell + (1/2))}{\sqrt{2Err'}}\Gamma(2\ell + 1)M_{p,\ell}\left(2i\sqrt{2E}r\right)W_{-p,\ell}\left(-2i\sqrt{2E}r'\right), \quad (11)$$

where $p = -\mathrm{i}Z/\sqrt{2E}$, while $M_{p,\ell}$ and $W_{-p,\ell}$ denote Whittaker functions.

Since we have the relation

$$\mathscr{L}_\beta C_\ell(r, r'; \beta) = G_\ell(r, r'; -E), \quad (12)$$

this proves our contention in the free-particle form equation (6) that $\mathscr{L}_\beta C_\ell(r, r'; \beta)$ also factorizes to read

$$\mathscr{L}_\beta C_\ell(r, r'; \beta) = A_\ell(r; E)B_\ell(r'; E), \quad (13)$$

where, apart from multiplying factors that also involve p, but not r and r',

$$A_\ell(r; E) = \frac{1}{\sqrt{r}}M_{p,\ell}(2\mathrm{i}\sqrt{2E}r) \quad (14)$$

while

$$B_\ell(r'; E) = \frac{1}{\sqrt{r'}}W_{-p,\ell}(-2\mathrm{i}\sqrt{2E}r'). \quad (15)$$

It is then straightforward from equations (14) and (15) to prove that $A_\ell = B_\ell$ for $\ell = 0$, when both reduce to the Kummer function $M(-\mathrm{i}Z/k, 0, 2\mathrm{i}kr)/\sqrt{r}$.

3. Introduction of 2D Coulomb potential: diagonal of Dirac density matrix, local density of states and imaginary part of Green function

In an earlier study on nonlinear scattering, March *et al*. [6] gave some attention to the introduction of a bare Coulomb potential $-Ze^2/r$ into a 2D, initially homogeneous electron assembly.

These workers gave a differential equation for the $\ell = 0$ component, say $N_0(r, E, Z)$, for the local density of states in the presence of the Coulomb potential. Their result for $N_0(r, E, Z)$ could be expressed in terms of the hypergeometric function ${}_1F_1$ as

$$\left.\frac{\partial\gamma_{\ell=0}(r, r'; E, Z)}{\partial E}\right|_{r'=r} \propto \left|{}_1F_1\left(\frac{iZ}{k} + \frac{1}{2}, 1, 2ikr\right)\right|^2; \quad k = \sqrt{2E}. \quad (16)$$

where $\gamma_{\ell=0}$ is the s-like component of the Dirac density matrix $\gamma(\mathbf{r}, \mathbf{r}'; E, Z)$. To relate to the free-electron limit discussed in some detail earlier, one can employ the identity

$$ {}_1F_1\left(p+\frac{1}{2}, 2p+1, 2iz\right) = \Gamma(p+1)\left(\frac{z}{2}\right)^{-p} \mathrm{e}^{iz} J_p(z) \tag{17} $$

in the case $p=0$. Then equation (16) reduces to the free-electron limit ($Z \to 0$ corresponding to $p=0$ in equation (17))

$$ \left.\frac{\partial \gamma_{\ell=0}(r, r'; E, Z)}{\partial E}\right|_{r'=r,\, Z=0} \propto J_0(\sqrt{2E}r)^2. \tag{18} $$

Thus we can write for the imaginary part of the 2D Green function for $\ell=0$ the result

$$ \mathrm{Im}\, G_{\ell=0}(r, r'; E, Z)|_{r'=r} \propto \left| {}_1F_1\left(\frac{iZ}{k}+\frac{1}{2}, 1, 2ikr\right)\right|^2. \tag{19} $$

This must evidently relate to $G_{\ell=0}(r, r'; E, Z)$ given in equation (26) of Inomata [5], and written in equation (11). Explicitly, this result reads (in atomic units)

$$ G_{\ell=0}(r, r'; E, Z) = \frac{-2\Gamma(p+(1/2))}{k\sqrt{rr'}}\ M_{p,0}(2ikr)\ W_{-p,0}(-2ikr'). \tag{20} $$

It remains to take the imaginary part of equation (20), after which, letting $r' \to r$ in $\mathrm{Im}\, G_{\ell=0}(r, r'; E, Z)$ one must recover the result (19).

Figure 1 shows the $\ell=0$ partial wave form of the imaginary part of the Green function for $Z=1$ and for the range of variables shown in the caption. Figure 2 is then for the more strongly scattering Coulomb potential with $Z=50$, the range of the variables again being given in the caption. Figure 2(a) is the counterpart of figure 1 for $Z=50$ now. However, in this strong scattering case, figure 2(b) depicts the nonlinear oscillatory behavior of $\mathrm{Im}\, G_{\ell=0}$ for $Z=50$ and two values of k.

We next note from Gradshteyn and Ryzhik [7] that the above Whittaker function $M_{p,\ell}$ is related to ${}_1F_1$ by

$$ M_{\lambda,\mu}(z) = z^{\mu+(1/2)} \mathrm{e}^{-z/2} {}_1F_1\left(\mu-\lambda+\frac{1}{2}, 2\mu+1, z\right). \tag{21} $$

When $\mu=0$, $\lambda=p$, and $z=2ikr$, this equation (21) becomes

$$ M_{p,0}(2ikr) = (2ikr)^{(1/2)} \mathrm{e}^{-ikr} {}_1F_1\left(-p+\frac{1}{2}, 1, 2ikr\right). \tag{22} $$

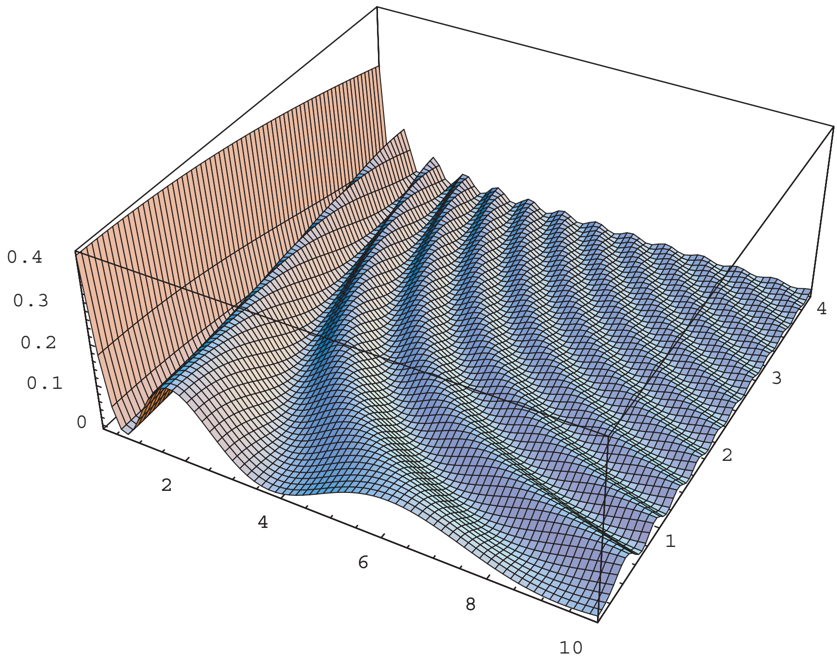


Figure 1. A plot of the RHS of equation (19) for the $\ell = 0$ partial wave form of the Green function for $Z = 1$, with $k \in [0.01, 4]$ and $r \in [0, 10]$.

With $p = -iZ/k$, this equation (16) can be used in equation (20) to remove the Whittaker function $M_{p,0}$ in favor of the hypergeometric function ${}_1F_1$ determining $\operatorname{Im} G_{\ell=0}(r, r'; E, Z)\big|_{r'=r}$ in equation (19). Hence it follows that

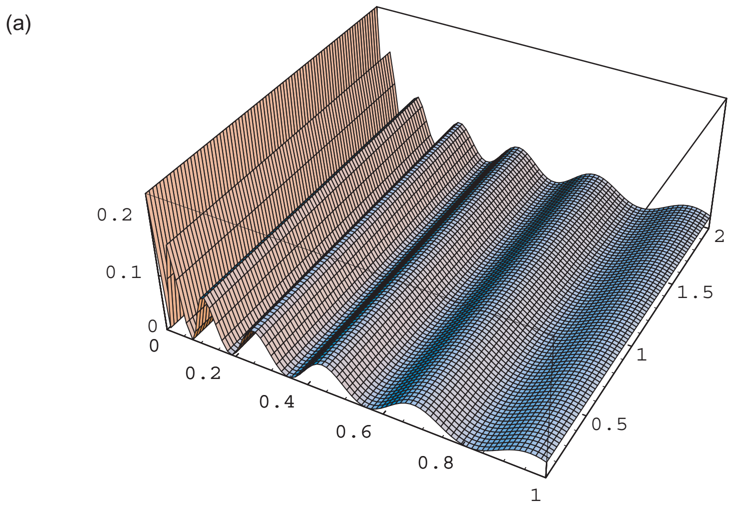
$$G_{\ell=0}(r, r'; E, Z) \propto {}_1F_1\left(-p + \frac{1}{2}, 1, 2ikr\right) W_{-p,0}(-2ikr'). \tag{23}$$

We can only take a limit in equation (23) as $r' \to r$ by removing the real part of $G_{\ell=0}(r, r'; E, Z)$. Then, $\operatorname{Im} G_{\ell=0}(r, r'; E, Z)\big|_{r'=r}$ must be given by equation (19) (see also figure 1).

3.1. *Form of density change $\Delta\rho(r, E, Z)$ due to potential $-Ze^2/r$ in 2D electron gas*

In the scattering theory set out by March *et al.* [6] a further result, which could be obtained without analyzing into partial waves, is for the change in density $\Delta\rho(\mathbf{r}, E, Z)$ induced by the bare Coulomb potential in 2D. Their result reads, at $\mathbf{r} = 0$:

$$\Delta\rho(0, E, Z) = \frac{E}{\pi} \tanh\left(\frac{Z\pi}{\sqrt{2E}}\right). \tag{24}$$



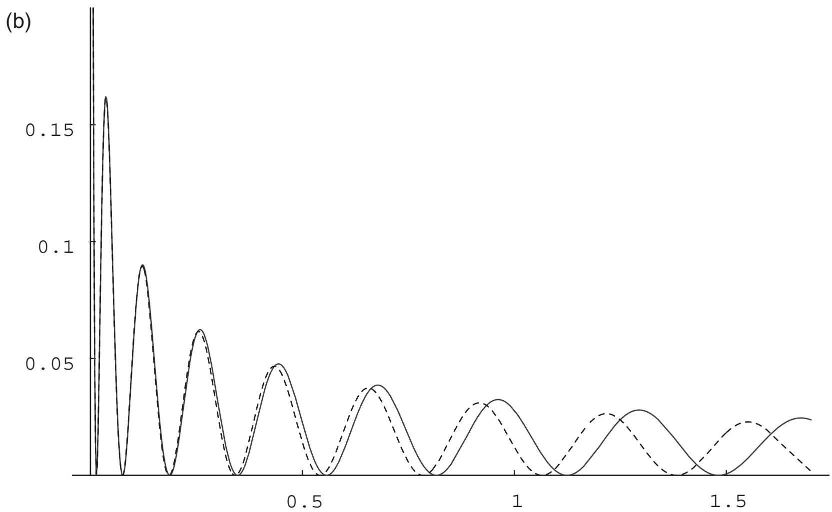


Figure 2. A plot of the RHS of equation (19) for the $\ell = 0$ partial wave form of the Green function for $Z = 50$. In (a) $k \in [0.1, 2]$ and $r \in [0, 1]$. In (b) the solid curve corresponds to $k = 0.4$ and the dashed line to $k = 4$.

This, to first order in Z, recovers the linear response result $Z\sqrt{E/2}$. Again, we are interested in the information that equation (24) contains concerning the imaginary part of $G(0, 0; E, Z)$ via

$$\frac{1}{\pi}\operatorname{Im}\Delta G(0, 0; E, Z) = \frac{\partial \Delta\rho(0, E, Z)}{\partial E}, \tag{25}$$

where ΔG stands for $G - G_{Z\to 0}$. The result in equation (16) must relate to equation (22) of Inomata when corrected for typographical errors, one at least being that $(r' - r'')^{1/2}$ should read $(r'r'')^{1/2}$. One must form $\Delta G(\mathbf{r}, \mathbf{r}' = 0; E, Z) = G - G_{Z\to 0}$ from equation (22) and then take the imaginary part as in equation (25). Only then can one pass to the diagonal limit $\mathbf{r} = \mathbf{r}' = 0$ required in equation (25).

4. Partial wave $\ell = 0$ component of Green function G(r, r′; E, Z) and limiting form as Z tends to zero

Work done by Inomata [5] has yielded a form for the Green function generated by the Coulomb potential $-Ze^2/r$ in 2D in terms of Whittaker functions M and W. The result of his equation (26) is written in equation (20). As $p = -\mathrm{i}Z/\sqrt{2E} \to 0$, we have the relations, see 9.235(1) and 9.235(2) of [7],

$$M_{0,0}(z) = \sqrt{z}\, I_0\left(\frac{z}{2}\right), \tag{26}$$

$$W_{0,0}(z) = \sqrt{\frac{z}{\pi}}\, K_0\left(\frac{z}{2}\right). \tag{27}$$

Hence, the free-electron limit $Z \to 0$ of equation (20) yields

$$G_{\ell=0}(r, r'; E)_{Z=0} = 4\, I_0(\mathrm{i}\sqrt{2E}r)K_0(-\mathrm{i}\sqrt{2E}r'). \tag{28}$$

Thus the free-particle limit of the Green function $G_{\ell=0}$ is known explicitly in terms of the modified Bessel functions I_0 and K_0.

Also, from earlier work in the body of this article, the imaginary part of $G_{\ell=0}(r, r'; E, Z)$ is determined on the diagonal $r' = r$ via the hypergeometric function as $\left|{}_1F_1(\mathrm{i}Z/k + (1/2), 1, 2\mathrm{i}kr)\right|^2$.

4.1. *Separation of free particle Green function into real and imaginary parts*

Using relations between Bessel functions and modified Bessel functions, we can write from equation (5):

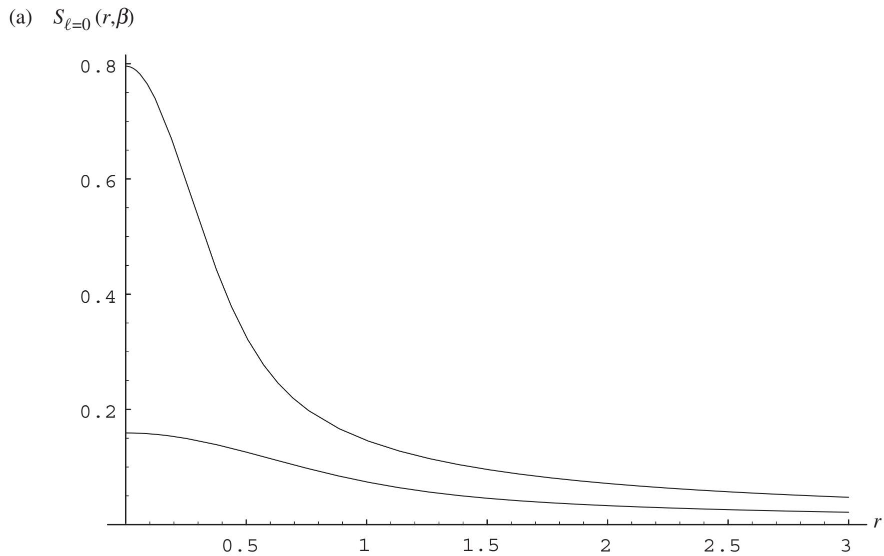
$$G_0(\mathbf{r}, \mathbf{r}'; E) = -\frac{1}{2} Y_0(\sqrt{2E}|\mathbf{r} - \mathbf{r}'|) + \frac{\mathrm{i}}{2} J_0(\sqrt{2E}|\mathbf{r} - \mathbf{r}'|). \tag{29}$$

For $Y_0(x)$ there is the known integral representation [8]

$$Y_0(x) = -\frac{2}{\pi}\int_0^\infty \cos(x\cosh t)\mathrm{d}t \quad (x > 0), \tag{30}$$

while for $J_0(x)$ the corresponding result is

$$J_0(x) = \frac{2}{\pi}\int_0^\infty \sin(x\cosh t)\mathrm{d}t \quad (x > 0). \tag{31}$$



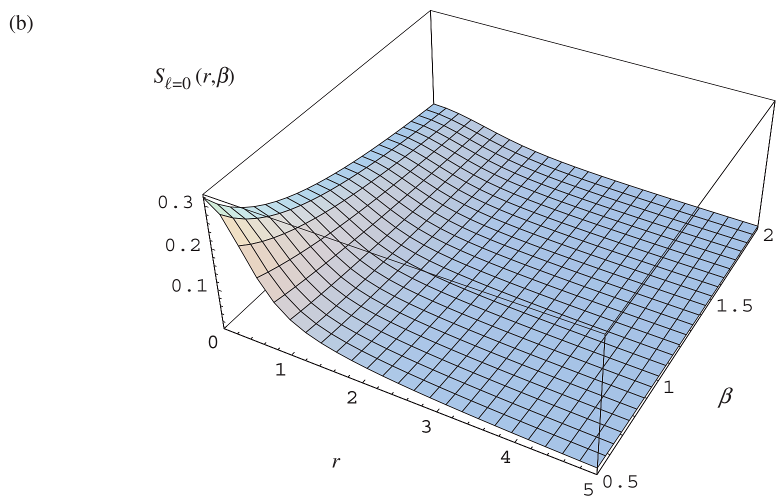


Figure 3. Graphic display of the Slater sum for the $\ell = 0$ partial wave: (a) as a function of r for $\beta = 0.2$ and 1; (b) in a 3D plot for $r \in [0, 5]$ and $\beta \in [0.5, 2]$.

Thus, from equations (29) to (31) one readily obtains

$$G_0(\mathbf{r}, \mathbf{r}'; E) = \frac{1}{\pi} \int_0^\infty \exp(\mathrm{i}\sqrt{2E}|\mathbf{r} - \mathbf{r}'| \cosh t)\mathrm{d}t, \tag{32}$$

and therefore

$$G_0(\mathbf{r}, \mathbf{r}'; -E) = \frac{1}{\pi} \int_0^\infty \exp(-\sqrt{2E}|\mathbf{r} - \mathbf{r}'| \cosh t)\mathrm{d}t, \tag{33}$$

which integrates to the result given in (5) by 8.432(1) of [7].

It is of interest here, because of the relation (4) between the canonical density matrix $C(\mathbf{r}, \mathbf{r}'; \beta)$ and $G(\mathbf{r}, \mathbf{r}'; -E)$, to record that after analyzing equation (3) into partial waves, the diagonal $S_{\ell=0}(r, \beta)$, the so-called Slater sum $C(\mathbf{r}, \mathbf{r}; \beta)$, can be calculated as

$$S_{\ell=0}(r, \beta) = \mathrm{e}^{-r^2/\beta} \frac{(I_0(r^2/\beta))}{2\pi\beta}. \tag{34}$$

This is related to the Feynman propagator for $\ell = 0$ by the transform $\beta \to \mathrm{i}t$. Figure 3 displays equation (34) for the different variable ranges displayed in the caption. This is the 2D counterpart for $\ell = 0$ of the 3D result of March and Murray [4] displayed below equation (6).

5. Summary and possible future directions

The main results of this study for the bare Coulomb potential $-Ze^2/r$ in two dimensions are:

- equation (19) for the imaginary part Im $G_{\ell=0}(r, r'; E, Z)|_{r'=r}$ for the 's-like' partial wave with $\ell = 0$ in equation (19); and
- for the imaginary part Im $\Delta G(0, 0; E, Z)$ due to the change ΔG in the Green function on switching on the Coulomb potential $-Ze^2/r$ to an initially homogeneous electron gas in 2D.

Additionally, as by-products of the present study, the free-particle Green function $G_0(\mathbf{r}, \mathbf{r}'; E)$ has been separated into its real and imaginary parts in equation (26), these parts being related by the Kramers–Krönig relation [9]. For the $\ell = 0$ component of the Slater sum, which in turn is the diagonal element of the canonical density matrix, equation (34) gives the closed analytic form in terms of the free-particle form times $I_0(r^2/\beta)$, which generalizes the result of March and Murray [4] following equation (6) for $\ell = 0$ to apply to two dimensions.

For future directions, it would be valuable if the $\ell = 0$ partial wave of the Green function of equation (20) could be separated into its real and imaginary parts. That would then effect the generalization of the free-electron limit equation (28) away from $Z = 0$.

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